



STIC Search Report

EIC 1700

STIC Database Tracking Number: EIC 1700

TO: Dawn Garrett
Location: REM 10C79
Art Unit : 1774
April 6, 2005

Case Serial Number: 10/729738

From: Les Henderson
Location: EIC 1700
REM 4B28 / 4A30
Phone: 571-272-2538

Leslie.henderson@uspto.gov

Search Notes

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: DAWN GARRETT Examiner #: 76107 Date: 3/23/2005
 Art Unit: 1774 Phone Number 302-1523 Serial Number: 10/729,738
 Mail Box and Bldg/Room Location: Roman 10C79 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Organic Electroluminescent Devices

Inventors (please provide full names):

JOSEPH DEATON, MARGARET HELBER, DAVID GIESEN

Earliest Priority Filing Date: 12/5/2003

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

SCIENTIFIC REFERENCE BR
Sci & Tech Inf. Ctr

Please search formulas

(1a), (1b), (2), (3), (4)

MAR 24 RECD

Pat. & T.M. Office

Thank you

STAFF USE ONLY

Searcher: LH

Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: _____

Date Completed: 4/6/05

Searcher Prep & Review Time: 3.0

Clerical Prep Time: 3.0

Online Time: 4.5

Type of Search

NA Sequence (#) _____

AA Sequence (#) _____

Structure (#) 2 _____

Bibliographic _____

Litigation _____

Fulltext _____

Patent Family _____

Other _____

Vendors and cost where applicable

STN \$ 553.19

Dialog _____

Questel/Orbit _____

Dr. Link _____

Lexis/Nexis _____

Sequence Systems _____

WWW/Internet _____

Other (specify) _____

=> d his

(FILE 'HOME' ENTERED AT 09:05:01 ON 06 APR 2005)

FILE 'LREGISTRY' ENTERED AT 09:05:17 ON 06 APR 2005

L1 STR

FILE 'REGISTRY' ENTERED AT 09:11:37 ON 06 APR 2005

L2 SCR 1841

L3 0 S L1 AND L2

FILE 'LREGISTRY' ENTERED AT 09:12:38 ON 06 APR 2005

L4 STR L1

FILE 'REGISTRY' ENTERED AT 09:16:53 ON 06 APR 2005

L5 45 S L4 AND L2

FILE 'LREGISTRY' ENTERED AT 09:21:52 ON 06 APR 2005

L6 STR L4

FILE 'REGISTRY' ENTERED AT 09:24:01 ON 06 APR 2005

L7 50 S L6 AND L2

L8 4402 S L6 AND L2 FUL

SAV L8 GAR738/A

FILE 'LREGISTRY' ENTERED AT 09:27:55 ON 06 APR 2005

L9 STR L6

FILE 'REGISTRY' ENTERED AT 09:29:53 ON 06 APR 2005

L10 3 S (L9 AND L2) SSS SAM SUB=L8

L11 55 S (L9 AND L2) SSS FUL SUB=L8

FILE 'LREGISTRY' ENTERED AT 09:34:20 ON 06 APR 2005

L12 STR L9

FILE 'REGISTRY' ENTERED AT 09:35:13 ON 06 APR 2005

L13 1 S L12 SSS SAM SUB=L8

L14 4 S L12 SSS FUL SUB=L8

SAV L11 GAR738A/A

SAV L14 GAR738B/A

FILE 'HCA' ENTERED AT 09:37:45 ON 06 APR 2005

L15 17 S L11

L16 0 S L14

FILE 'CAOLD' ENTERED AT 09:41:08 ON 06 APR 2005

L17 0 S L11

L18 0 S L14

FILE 'HCAPLUS' ENTERED AT 09:41:44 ON 06 APR 2005

L19 18 S L11

S L4

FILE 'REGISTRY' ENTERED AT 09:42:22 ON 06 APR 2005

FILE 'HCAPLUS' ENTERED AT 09:42:23 ON 06 APR 2005

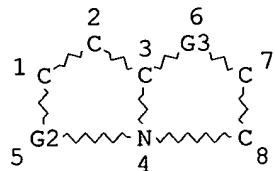
L20 1 S L14

L21 17 S L19 NOT L20

FILE 'CAPLUS' ENTERED AT 09:44:05 ON 06 APR 2005
 L22 18 S L11
 L23 1 S L14
 L24 18 S L19 AND L22

FILE 'HCAPLUS' ENTERED AT 09:45:16 ON 06 APR 2005

=> d que stat 120
 L2 SCR 1841
 L6 STR



VAR G2=IR/RH/RU/OS/PT/PD

REP G3=(1-2) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

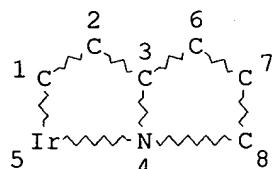
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L8 4402 SEA FILE=REGISTRY SSS FUL L6 AND L2
 L12 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L14 4 SEA FILE=REGISTRY SUB=L8 SSS FUL L12
 L20 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L14

=> d 120 1 ibib abs hitstr hitind

L20 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:212410 HCAPLUS

TITLE: Organometallic complex for organic
electroluminescent device

INVENTOR(S): Inoue, Eiko; Tokuda, Atsushi; Yamazaki, Hiroko;

PATENT ASSIGNEE(S): Seo, Satoshi
 SOURCE: Semiconductor Energy Laboratory Co., Ltd., Japan
 Jpn. Kokai Tokkyo Koho, 37 pp.
 CODEN: JKXXAF

DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005060374	A2	20050310	JP 2004-217219	200407 26
PRIORITY APPLN. INFO.:			JP 2003-280667	A 200307 28

GI

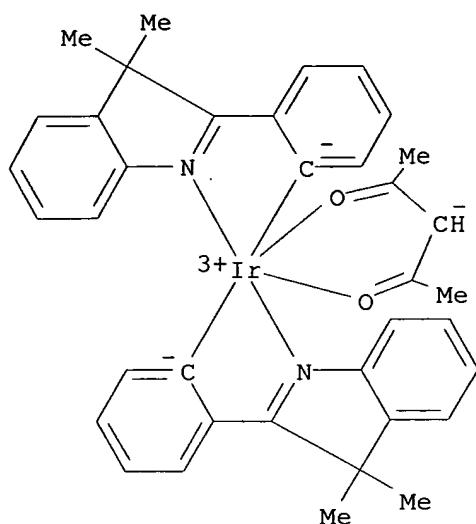
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Disclosed are organometallic complexes, suited for use as a phosphorescent substance in an organic electroluminescent device, represented by I [R1-4 = H, halo, alkyl, etc.; R5 and R6 = H and alkyl; Ar = arylene, and heterocyclic residue; M = Group VIII element; n = 1 or 2; L = monoanion ligand having diketone structure, monoanionic bidentate chelate ligand having carboxylic group, and monoanionic bidentate chelate ligand having phenol hydroxy group], II [R1-8 = H, halo, alkyl, etc.; R9 and R10 = H and alkyl; Ar = arylene, and heterocyclic residue; M = Group VIII element; n = 1 or 2; L = monoanion ligand having diketone structure, monoanionic bidentate chelate ligand having carboxylic group, and monoanionic bidentate chelate ligand having phenol hydroxy group], III, and IV [R1-10 = H, halo, alkyl, etc.; Ar = arylene, and heterocyclic residue; M = Group VIII element; n = 1 or 2; L = monoanion ligand having diketone structure, monoanionic bidentate chelate ligand having carboxylic group, and monoanionic bidentate chelate ligand having phenol hydroxy group].

IT 847606-35-3P 847606-37-5P
 RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (phosphorescent organometallic complex for organic electroluminescent device)

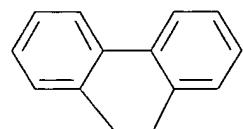
RN 847606-35-3 HCAPLUS

CN INDEX NAME NOT YET ASSIGNED

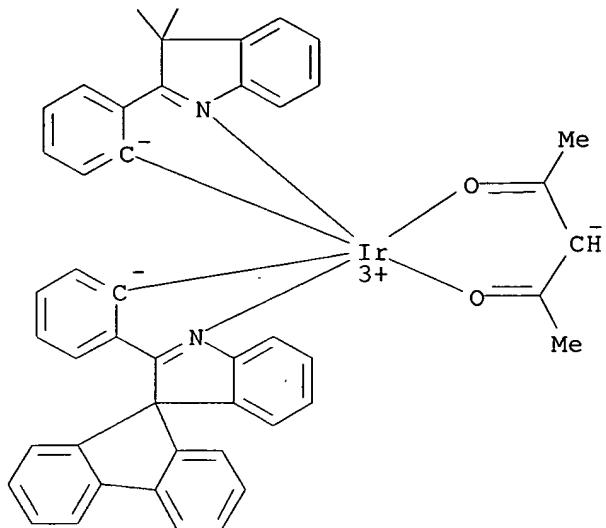


RN 847606-37-5 HCPLUS
CN INDEX NAME NOT YET ASSIGNED

PAGE 1-A



PAGE 2-A

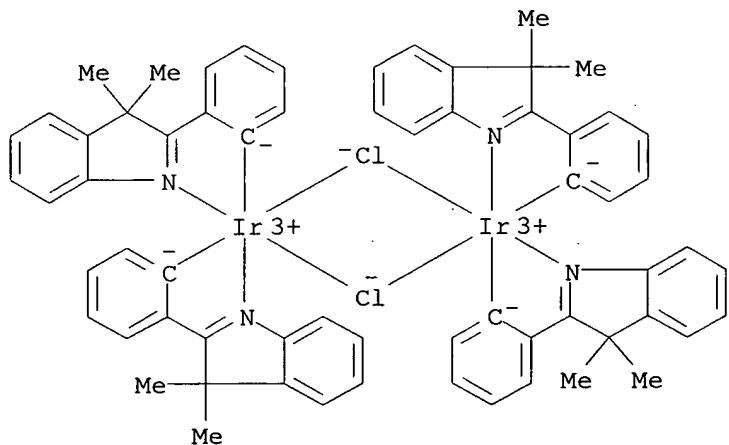


IT 847606-34-2P 847606-36-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (phosphorescent organometallic complex for organic
 electroluminescent device)

RN 847606-34-2 HCAPLUS

CN INDEX NAME NOT YET ASSIGNED



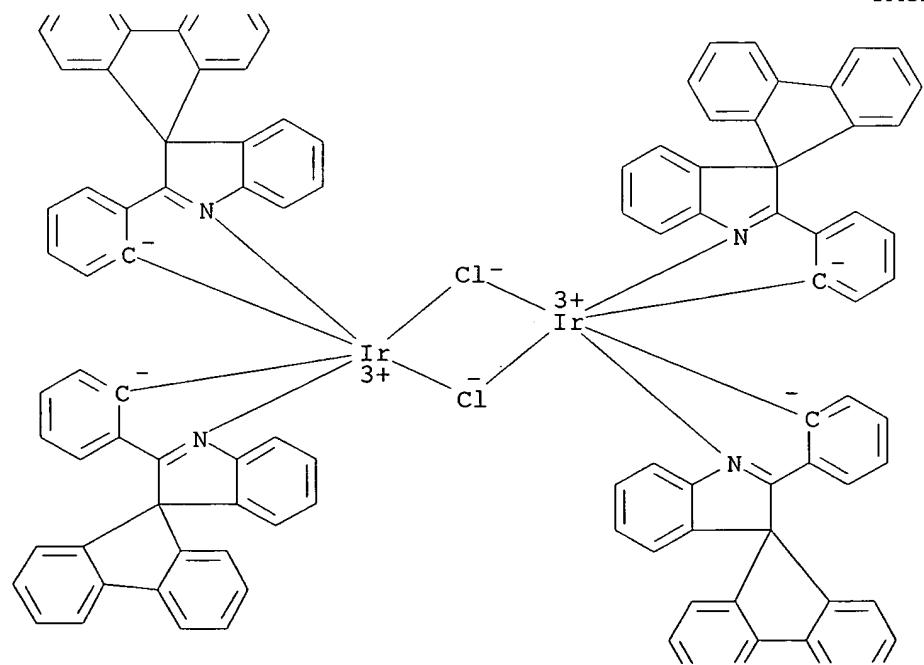
RN 847606-36-4 HCAPLUS

CN INDEX NAME NOT YET ASSIGNED

PAGE 1-A

// \ \ / \ \ \

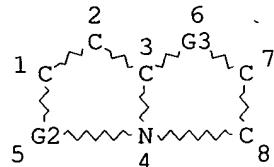
PAGE 2-A



PAGE 3-A

IC ICM C07F015-00
 ICS C07D209-08; C09K011-06; H05B033-14
 CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
 Section cross-reference(s): 29, 74, 78
 IT 847606-35-3P 847606-37-5P
 RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (phosphorescent organometallic complex for organic electroluminescent device)
 IT 1603-73-2P, 9-Benzoylfluorene 4643-66-7P 6636-32-4P
 847606-34-2P 847606-36-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (phosphorescent organometallic complex for organic electroluminescent device)

=> d que stat l21
 L2 SCR 1841
 L6 STR

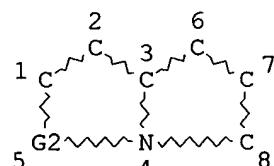


VAR G2=IR/RH/RU/OS/PT/PD
 REP G3=(1-2) C

NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE
 L8 4402 SEA FILE=REGISTRY SSS FUL L6 AND L2
 L9 STR



VAR G2=IR/RH/RU/OS/PT/PD

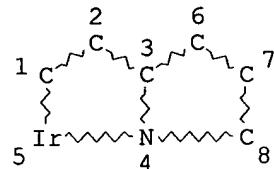
NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L11 55 SEA FILE=REGISTRY SUB=L8 SSS FUL (L9 AND L2)
L12 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L14 4 SEA FILE=REGISTRY SUB=L8 SSS FUL L12
L19 18 SEA FILE=HCAPLUS ABB=ON PLU=ON L11
L20 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L14
L21 17 SEA FILE=HCAPLUS ABB=ON PLU=ON L19 NOT L20

=> d l21 1-17 ibib abs hitstr hitind

L21 ANSWER 1 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:984268 HCAPLUS

DOCUMENT NUMBER: 141:157273

TITLE: Bioorganometallic coordination compounds:
synthesis and structures of transition metal
complexes containing tropidinyl and tropidine
ligands

AUTHOR(S): Tamm, Matthias; Kunst, Andreas; Hahn, F.
Ekkehardt; Pape, Tania; Froehlich, Roland

CORPORATE SOURCE: Anorganisch-Chemisches Institut, Technischen
Universitaet Muenchen, Munich, Germany

SOURCE: Zeitschrift fuer Anorganische und Allgemeine
Chemie (2003), 629(12-13), 2408-2414
CODEN: ZAACAB; ISSN: 0044-2313

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:157273

AB Deprotonation of the alkene tropidine (1), or 8-methyl-8-azabicyclo[3.2.1]oct-2-ene, resp., with BuNa gave a Na salt containing the tropidinyl anion (2). Treatment with Me₃SnCl affords 4-trimethylstannyltropidine (3), which can be used as a starting material for the preparation of tropidinyl transition metal complexes. [(2)M(CO)₃] (M = Mn, 4a; M = Re, 4b) can be obtained from the reaction of 3 with [M(CO)₅Br], whereas the reaction with [Ru(PPh₃)₃Cl₂] gives [(2)Ru(PPh₃)₂Cl] (5). In 4 and 5, the tropidinyl ligand 2 is

coordinated through the bridging N atom as well as through the three allylic C atoms and serves as a $2\sigma/4\pi$ -electron donor. It can thus be regarded as an analog of the cyclopentadienyl ligand. The reaction of the chloro complex 5 with super hydride, $\text{Li}[\text{BEt}_3\text{H}]$, affords the hydride $[(2)\text{Ru}(\text{PPh}_3)_2\text{H}]$ (6). On crystallization of 6, the peroxy complex $[(1)\text{Ru}(\text{PPh}_3)_2(\text{O}_2)]$ (7) containing the tropidine ligand 1 is formed. 4A, 5· CH_2Cl_2 and 7 were characterized by single-crystal x-ray diffraction analyses.

IT

728930-17-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

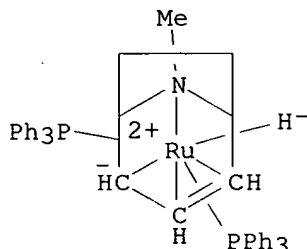
(conversion to peroxy complex during crystallization; synthesis and/or structures of manganese, rhenium and ruthenium complexes containing tropidinyl or tropidine ligands)

RN

728930-17-4 HCPLUS

CN

Ruthenium, hydro $[(2,3,4-\eta)-\text{rel}-(1R,4S)-8\text{-methyl-8-azabicyclo[3.2.1]oct-3-en-2-yl-}\kappa\text{N}]\text{bis}(\text{triphenylphosphine})$ -, stereoisomer (9CI) (CA INDEX NAME)



IT

728930-18-5P 729597-63-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

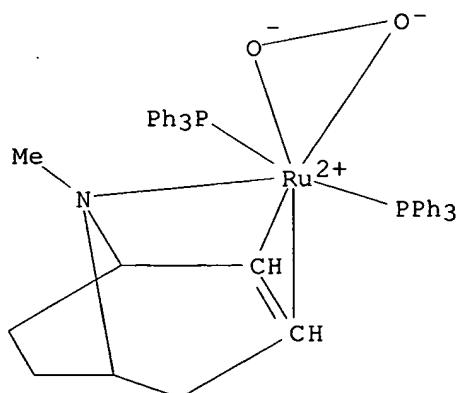
(crystal structure; synthesis and/or structures of manganese, rhenium and ruthenium complexes containing tropidinyl or tropidine ligands)

RN

728930-18-5 HCPLUS

CN

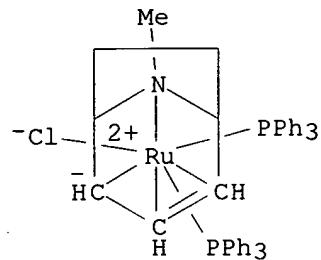
Ruthenium, $[(2,3-\eta)-\text{rel}-(1R,5S,8R)-8\text{-methyl-8-azabicyclo[3.2.1]oct-2-ene-}\kappa\text{N}]\text{peroxybis}(\text{triphenylphosphine})$ -, stereoisomer (9CI) (CA INDEX NAME)



RN 729597-63-1 HCAPLUS
 CN Ruthenium, chloro[(2,3,4- η)-rel-(1R,5S)-8-methyl-8-azabicyclo[3.2.1]oct-3-en-2-yl- κ N]bis(triphenylphosphine)-, stereoisomer, compd. with dichloromethane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 728930-16-3
 CMF C44 H42 Cl N P2 Ru
 CCI CCS



CM 2

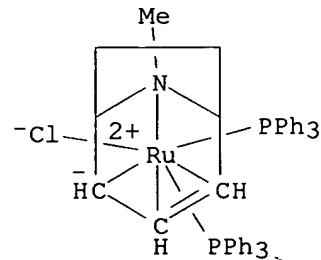
CRN 75-09-2
 CMF C H2 Cl2

Cl—CH₂—Cl

IT 728930-16-3P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)
 (mol. structure, conversion to hydrido complex; synthesis and/or
 structures of manganese, rhenium and ruthenium complexes containing
 tropidinyl or tropidine ligands)

RN 728930-16-3 HCAPLUS
 CN Ruthenium, chloro[(2,3,4- η)-rel-(1R,5S)-8-methyl-8-azabicyclo[3.2.1]oct-3-en-2-yl- κ N]bis(triphenylphosphine)-, stereoisomer (9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75

IT **728930-17-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (conversion to peroxy complex during crystallization; synthesis and/or
 structures of manganese, rhenium and ruthenium complexes containing
 tropidinyl or tropidine ligands)

IT **728930-18-5P 728930-19-6P 729597-63-1P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP
 (Preparation)
 (crystal structure; synthesis and/or structures of manganese,
 rhenium and ruthenium complexes containing tropidinyl or tropidine
 ligands)

IT **728930-16-3P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)
 (mol. structure, conversion to hydrido complex; synthesis and/or
 structures of manganese, rhenium and ruthenium complexes containing
 tropidinyl or tropidine ligands)

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L21 ANSWER 2 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:772148 HCAPLUS

DOCUMENT NUMBER: 137:295098

TITLE: Preparation of orthopalladated phenylpyrrole
 complexes as catalysts

INVENTOR(S): Plant, Andrew; Grosser, Rolf

PATENT ASSIGNEE(S): Bayer AG, Germany

SOURCE: Ger. Offen., 22 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

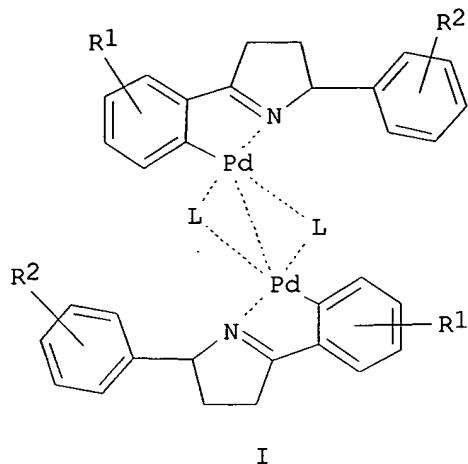
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10117674	A1	20021010	DE 2001-10117674	200104 09
WO 2002081489	A1	20021017	WO 2002-EP3842	200204 08

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH,
 CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD,
 GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ,
 LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ,
 NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,
 TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE,
 CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT,
 SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
 SN, TD, TG

PRIORITY APPLN. INFO.: DE 2001-10117674 A

200104
09

OTHER SOURCE(S): CASREACT 137:295098; MARPAT 137:295098
GI

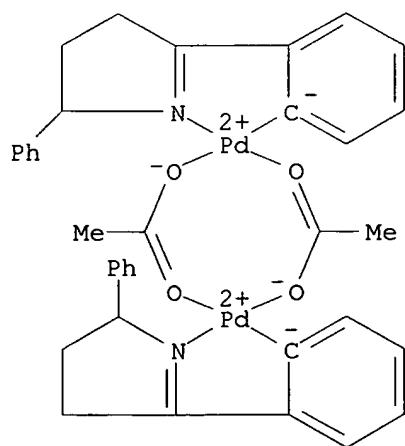


AB The preparation of new title palladium complexes I ($R_1 = H$, alkoxy, dialkylamino, Ph, $R_2 = H$, alkyl, alkoxy, dialkylamino, etc., $L = OCOC_2H_5$, $OCOC_2F_5$, Cl, Br, etc.), useful as catalysts, is described. Thus, orthopalladation of 2,5-diphenyl-3,4-dihydro-2H-pyrrole with $Pd(OAc)_2$ in THF gave 100% title compound, I ($R_1, R_2 = H$, $L = acetyl$).

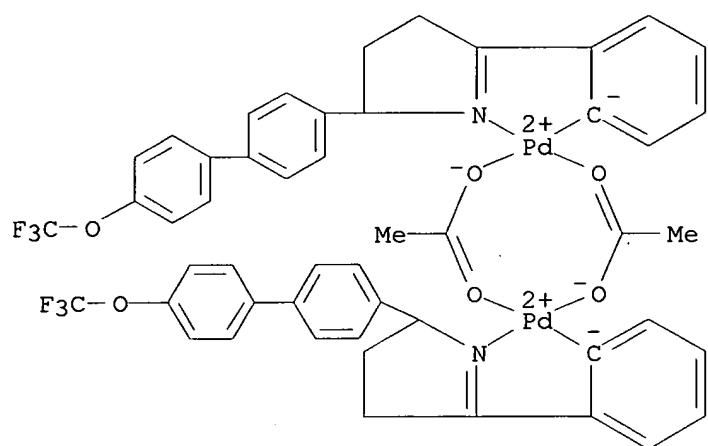
IT **467421-49-4P**
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(crystal structure; preparation as coupling reaction catalyst)

RN 467421-49-4 HCAPLUS

CN Palladium, *rel*-bis[μ -(acetato- κ O: κ O')]bis[2-[(2R)-3,4-dihydro-2-phenyl-2H-pyrrol-5-yl- κ N]phenyl- κ C]di-, stereoisomer (9CI) (CA INDEX NAME)

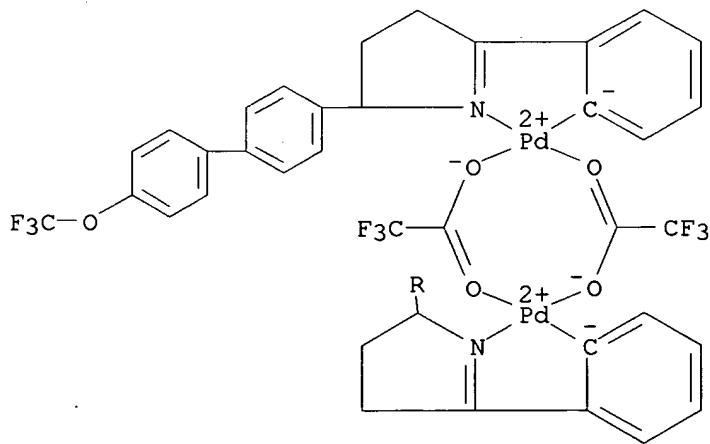


IT 467421-50-7P 467421-51-8P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)
(preparation as coupling reaction catalyst)
RN 467421-50-7 HCAPLUS
CN Palladium, bis[μ-(acetato-κO:κO')]bis[2-[3,4-dihydro-
2-[4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]-2H-pyrrol-5-yl-
κN]phenyl-κC]di- (9CI) (CA INDEX NAME)

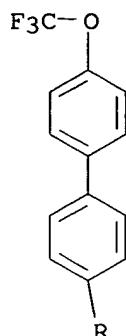


RN 467421-51-8 HCPLUS
CN Palladium, bis[2-[3,4-dihydro-2-[4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]-2H-pyrrol-5-yl- κ N]phenyl- κ C]bis[μ -(trifluoroacetato- κ O: κ O')]di- (9CI) (CA INDEX NAME)

PAGE 1-A

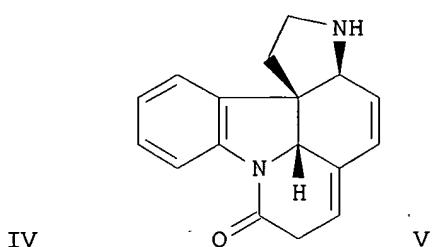
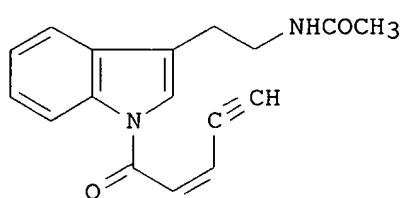
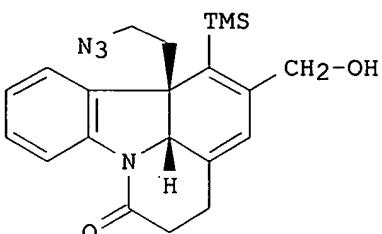
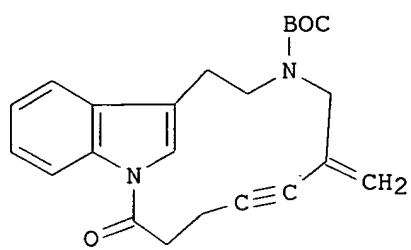


PAGE 2-A



IC ICM C07F015-00
 CC 29-13 (Organometallic and Organometalloidal Compounds)
 IT **467421-49-4P**
 RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (crystal structure; preparation as coupling reaction catalyst)
 IT **467421-50-7P 467421-51-8P**
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (preparation as coupling reaction catalyst)

L21 ANSWER 3 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2001:627687 HCAPLUS
 DOCUMENT NUMBER: 135:358077
 TITLE: Approaches to the Synthesis of (\pm)-Strychnine
 via the Cobalt-Mediated [2 + 2 + 2]
 Cycloaddition: Rapid Assembly of a Classic
 Framework
 AUTHOR(S): Eichberg, Michael J.; Dorta, Rosa L.; Grotjahn,
 Douglas B.; Lamottke, Kai; Schmidt, Martin;
 Vollhardt, K. Peter C.
 CORPORATE SOURCE: Center for New Directions in Organic Synthesis
 Department of Chemistry and the Chemical
 Sciences Division, Lawrence Berkeley National
 Laboratory, University of California at
 Berkeley, Berkeley, CA, 94720-1460, USA
 SOURCE: Journal of the American Chemical Society (2001),
 123(38), 9324-9337
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 135:358077
 GI



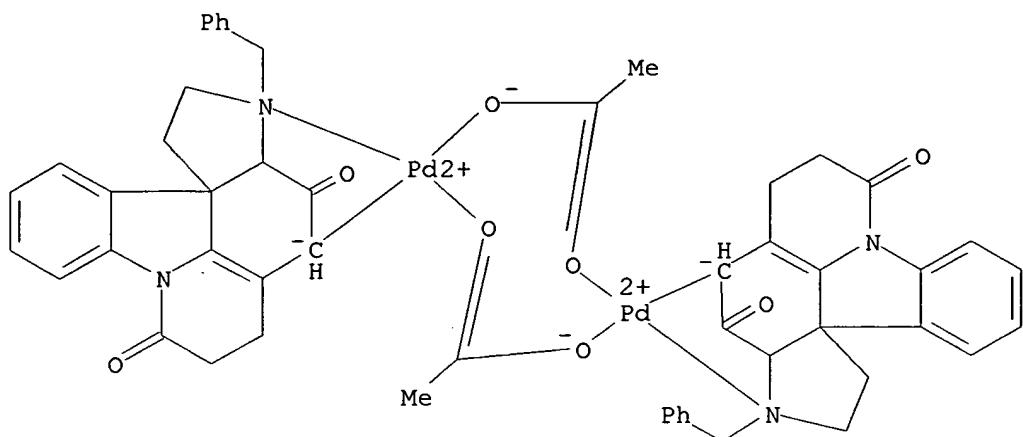
AB Five synthetic approaches to racemic strychnine (I), with the cobalt-mediated [2+2+2] cycloaddn. of alkynes to indoles as the key step, are described. These include the generation and attempted cyclization of macrocycle II and the synthesis of dihydrocarbazoles, e.g. III and their elaboration to pentacyclic structures via a conjugate addition, dipolar cycloaddn., and propellane-to-spirofused skeletal rearrangement, resp. Finally, the successful total synthesis of I is discussed. The development of a short, highly convergent route (14 steps in the longest linear sequence) is highlighted by the cyclization of enynoylindole IV with acetylene and formal intramol. 1,8-conjugate addition to form pentacycle V. Numerous attempts toward the formation of the piperidine ring of I from vinyl iodide 56 were made and its successful formation via palladium-, nickel-, and radical-mediated processes is described.

IT **371246-17-2P 371246-18-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(approaches to the synthesis of (\pm)-strychnine via cobalt-mediated [2+2+2] cycloaddn.)

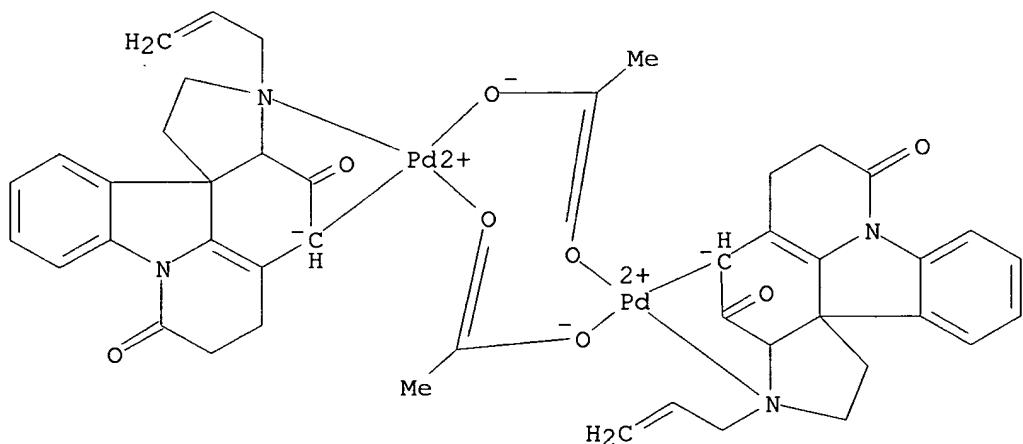
RN 371246-17-2 HCPLUS

CN Palladium, bis[μ -(acetato- κ O: κ O')]bis[1,2,3,10,11,12, 13,13a-octahydro-9,13-dioxo-1-(phenylmethyl)-9H-pyrido[1,2,3-1m]pyrrolo[2,3-d]carbazol-12-yl- κ C12, κ N1]di- (9CI) (CA INDEX NAME)



RN 371246-18-3 HCAPLUS

CN Palladium, bis[μ-(acetato-κO:κO')]bis[1,2,3,10,11,12,13,13a-octahydro-9,12-dioxo-1-(2-propenyl)-9H-pyrido[1,2,3-1m]pyrrolo[2,3-d]carbazol-12-yl-κC12,κN1]di- (9CI) (CA INDEX NAME)



CC 31-5 (Alkaloids)

Section cross-reference(s): 29

IT 141081-25-6P 155206-88-5P 293315-80-7P 293315-81-8P

371246-03-6P 371246-07-0P 371246-12-7P 371246-15-0P

371246-16-1P **371246-17-2P 371246-18-3P**

371246-19-4P 371246-23-0P 371246-24-1P 371246-25-2P

371246-26-3P 371246-27-4P 371246-29-6P 371246-30-9P

371246-31-0P 371246-33-2P 371246-34-3P 371246-35-4P

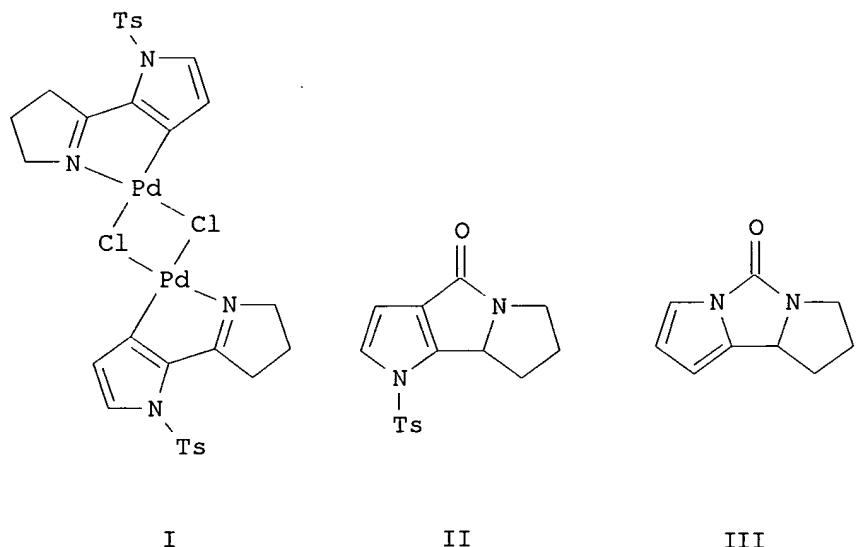
371246-36-5P 371246-38-7P 372161-57-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(approaches to the synthesis of (±)-strychnine via cobalt-mediated [2+2+2] cycloaddn.)

REFERENCE COUNT: 175 THERE ARE 175 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 4 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2000:709593 HCAPLUS
 DOCUMENT NUMBER: 134:207935
 TITLE: Cyclopalladation in pyrroles - Some initiating studies
 AUTHOR(S): Zhao, Yuekun; Helliwell, Madeleine; Joule, John A.
 CORPORATE SOURCE: Chemistry Department, The University of Manchester, Manchester, M13 9PL, UK
 SOURCE: ARKIVOC [online computer file] (2000), 1(3), 352-363
 CODEN: AKVCFI
 URL: <http://www.arkat.org/arkat/journal/Issue3/onweb21/gj21.htm>
 PUBLISHER: ARKAT Foundation
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:207935
 GI

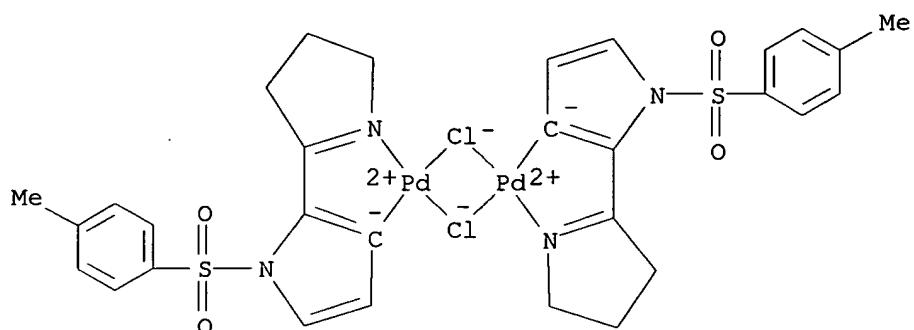


AB Cyclopalladation reactions of 3,4-dihydro-5-(1-(4-methylphenylsulfonyl)pyrrolyl)pyrrole with Pd(OAc)₂/AcOH gave palladacycle derivs., e.g., I, which were subsequently depalladohalogenated (X₂/NaOAc/CH₂Cl₂, X = Br, I) and converted by t-BuLi to tricyclic lactam II and by carbonyl diimidazole/NaH to tricyclic urea derivative III.

IT 328903-92-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (preparation and halogenation reactions of)

RN 328903-92-0 HCAPLUS

CN Palladium, di- μ -chlorobis[2-(3,4-dihydro-2H-pyrrol-5-yl- κ N)-1-[(4-methylphenyl)sulfonyl]-1H-pyrrol-3-yl- κ C]di-, stereoisomer (9CI) (CA INDEX NAME)



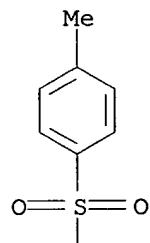
IT 328903-91-9B

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (preparation and nucleophilic substitution reactions of)

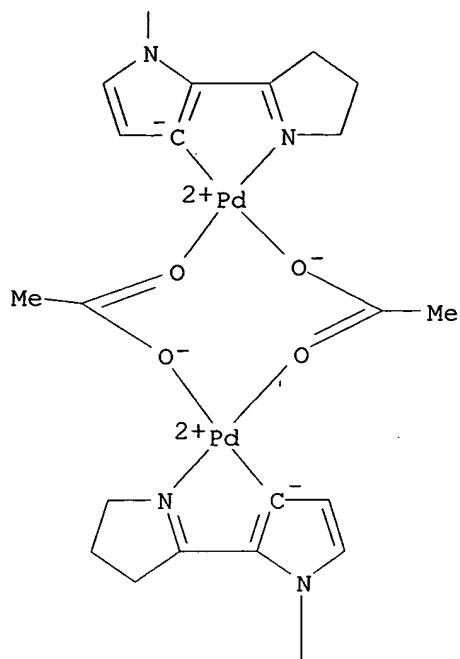
RN 328903-91-9 HCAPLUS

CN Palladium, bis[μ-(acetato-κO:κO')]bis[2-(3,4-dihydro-2H-pyrrol-5-yl-κN)-1-[(4-methylphenyl)sulfonyl]-1H-pyrrol-3-yl-κC]di-, stereoisomer (9CI) (CA INDEX NAME)

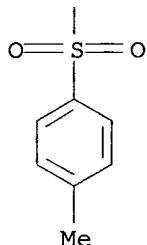
PAGE 1-A



PAGE 2-A



PAGE 3-A



CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 28

IT **328903-92-0P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (preparation and halogenation reactions of)

IT **328903-91-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (preparation and nucleophilic substitution reactions of)

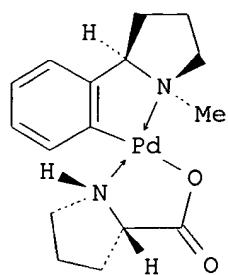
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L21 ANSWER 5 OF 17 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:159352 HCPLUS

DOCUMENT NUMBER: 132:321957

TITLE: Kinetic resolution of N-methyl-2-phenyl-pyrrolidine by cyclopalladation in the presence of an optically active base
 AUTHOR(S): Dunina, V. V.; Kuz'mina, L. G.; Razmyslova, E. D.; Kislyi, V. P.
 CORPORATE SOURCE: M. V. Lomonosov Moscow State University, Moscow, 119899, Russia
 SOURCE: Chemistry of Heterocyclic Compounds (New York) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2000), Volume 1999, 35(8), 1001-1011
 CODEN: CHCCAL; ISSN: 0009-3122
 PUBLISHER: Consultants Bureau
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



I

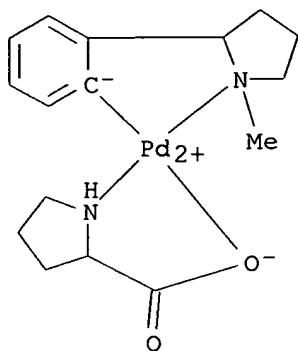
AB The possibility of the kinetic resolution of the racemic C*-chiral ligand in the course of its orthopalladation in the presence of an optically active base was shown for the first time using a tertiary heterocyclic amine as the ligand. The absolute configuration of the C*-stereocenter in the predominant enantiomer of the dimeric complex I was established by the x-ray diffraction of (S)-prolinate derivative

IT 150952-81-1P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)
 (crystal structure; kinetic resolution of methylphenylpyrrolidine by cyclopalladation in presence of optically active base)

RN 150952-81-1 HCAPLUS

CN Palladium, [2-[(1S,2S)-1-methyl-2-pyrrolidinyl- κ N]phenyl- κ C][(1R)-L-prolinato- κ N1, κ O2]-, (SP-4-4)- (9CI)
 (CA INDEX NAME)

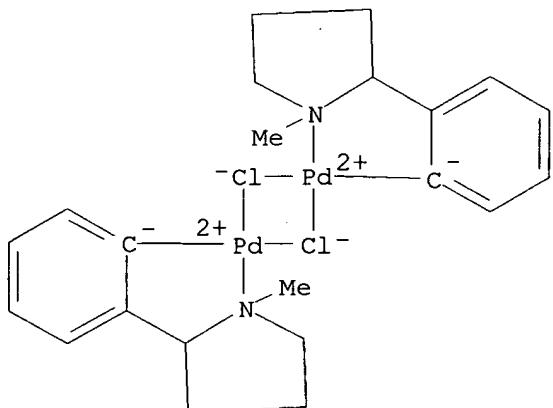


IT 267003-56-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (kinetic resolution of methylphenylpyrrolidine by cyclopalladation
 in presence of optically active base)

RN 267003-56-5 HCPLUS

CN Palladium, di- μ -chlorobis[2-(1-methyl-2-pyrrolidinyl-
 κ N)phenyl- κ C]di-, stereoisomer (9CI) (CA INDEX NAME)

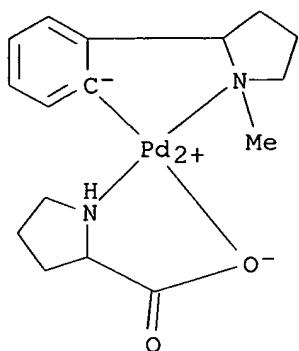


IT 151062-05-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (kinetic resolution of methylphenylpyrrolidine by cyclopalladation
 in presence of optically active base)

RN 151062-05-4 HCPLUS

CN Palladium, [2-[(1S,2S)-1-methyl-2-pyrrolidinyl- κ N]phenyl- κ C][(1S)-L-prolinato- κ N1, κ O2]-, (SP-4-4)- (9CI)
 (CA INDEX NAME)

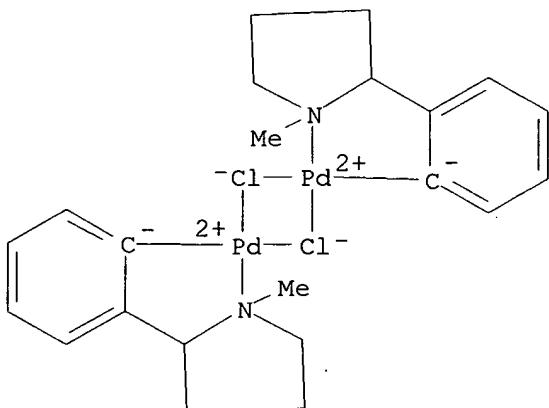


IT 267003-23-6P 267003-50-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (kinetic resolution of methylphenylpyrrolidine by cyclopalladation
 in presence of optically active base)

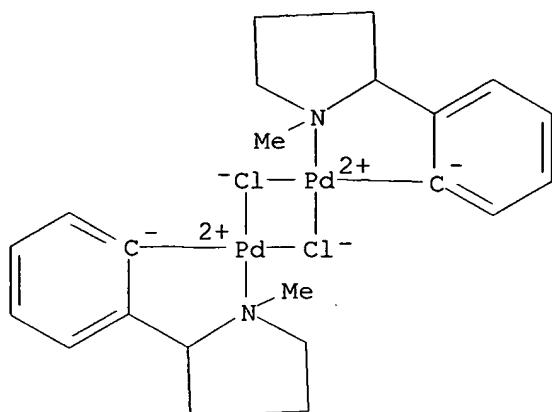
RN 267003-23-6 HCPLUS

CN Palladium, di- μ -chlorobis[2-[(1S,2S)-1-methyl-2-pyrrolidinyl-
 κ N]phenyl- κ C]di-, stereoisomer (9CI) (CA INDEX NAME)



RN 267003-50-9 HCPLUS

CN Palladium, di- μ -chlorobis[2-[(1R,2R)-1-methyl-2-pyrrolidinyl-
 κ N]phenyl- κ C]di-, stereoisomer (9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75

IT 150952-81-1P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)
 (crystal structure; kinetic resolution of methylphenylpyrrolidine by
 cyclopalladation in presence of optically active base)

IT 121378-60-7, Potassium S-proline 161876-10-4 264197-10-6

267003-56-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (kinetic resolution of methylphenylpyrrolidine by cyclopalladation
 in presence of optically active base)

IT 84591-31-1P 151062-05-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (kinetic resolution of methylphenylpyrrolidine by cyclopalladation
 in presence of optically active base)

IT 267003-23-6P 267003-50-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (kinetic resolution of methylphenylpyrrolidine by cyclopalladation
 in presence of optically active base)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L21 ANSWER 6 OF 17 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:561925 HCPLUS

DOCUMENT NUMBER: 131:322758

TITLE: Metal complexes of biologically important
 ligands. Part 121. Ortho-palladated enolates
 from N-(diphenylmethylene) Schiff bases of
 α -amino acid esters as ambivalent
 1,3-dipoles in [2+3] cycloadditions. Structures
 of a series of cycloadducts. Structures

AUTHOR(S): Schreiner, Bernhard; Urban, Reinhold;
 Zografas, Anastassios; Sunkel, Karlheinz;

CORPORATE SOURCE: Polborn, Kurt; Beck, Wolfgang
 Institut Anorganische Chemie,
 Ludwig-Maximilians-Univ., Munich, D-81377,
 Germany

SOURCE: Zeitschrift fuer Naturforschung, B: Chemical
 Sciences (1999), 54(8), 970-988

CODEN: ZNBSEN; ISSN: 0932-0776

PUBLISHER: Verlag der Zeitschrift fuer Naturforschung

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 131:322758

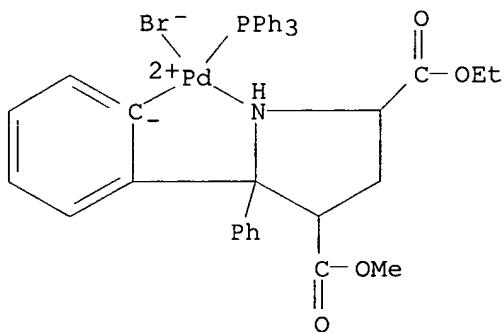
AB Enolates of ortho-palladated N-(diphenylmethylene) Schiff bases from glycine esters ($R_3Pd[C_6H_4CPh:NCR_1:C(OR)O]$) were isolated and are ambivalent 1,3-dipoles in [2+3] cycloaddns. $(NC)_2C:C(CN)_2$, $MeO_2CC.tpbond.CCO_2Me$, $MeO_2CN:NCO_2Me$, Ph_2CS , 2,2,4,4-tetramethyl-3-thioxocyclobutanone, 1,2,4-triazoline-3,5-dione, Ph_2CCO , and $PhNCO$ are added at the Pd and the enolate α -C atoms, whereas $HC.tpbond.CCO_2Me$, $CH_2:CHCO_2Me$, and Me maleate and Me fumarate form [2+3] cycloadducts with the α -C and the imino C atoms of the enolates under mild conditions. The structures of 7 cycloadducts were determined by x-ray diffraction anal.

IT 248282-28-2P 248282-30-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(crystal structure; ortho-palladated enolates from Schiff bases of amino acid esters as dipoles in [2+3] cycloaddn. reactions)

RN 248282-28-2 HCPLUS

CN Palladium, bromo[rel-2-[(1R,2R,3R,5R)-5-(ethoxycarbonyl)-3-(methoxycarbonyl)-2-phenyl-2-pyrrolidinyl- κ N]phenyl- κ C](triphenylphosphine)-, (SP-4-4)- (9CI) (CA INDEX NAME)

RN 248282-30-6 HCPLUS

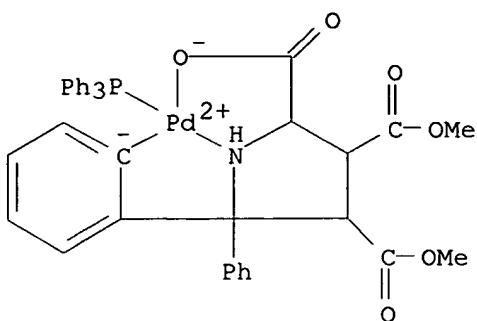
CN Palladium, [rel-3,4-dimethyl (1R,2R,3R,4R,5R)-5-(phenyl- κ C2)-5-phenyl-2,3,4-pyrrolidinetricarboxylato(2-)- κ N1, κ O2](triphenylphosphine)-, (SP-4-3)-, compd. with dichloromethane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 248282-29-3

CMF C39 H34 N O6 P Pd

CCI CCS

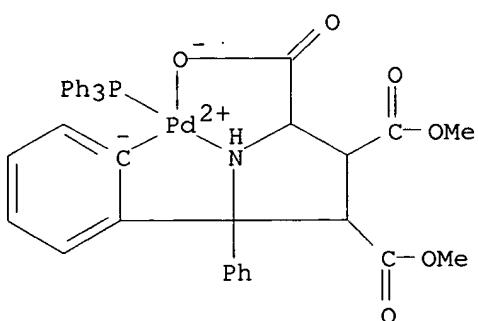


CM 2

CRN 75-09-2
CMF C H2 Cl2Cl-CH₂-ClIT 248282-29-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

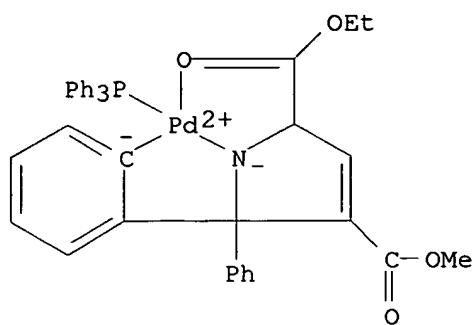
(mol. structure; ortho-palladated enolates from Schiff bases of amino acid esters as dipoles in [2+3] cycloaddn. reactions)

RN 248282-29-3 HCPLUS

CN Palladium, [rel-3,4-dimethyl (1R,2R,3R,4R,5R)-5-(phenyl- κ C2)-5-phenyl-2,3,4-pyrrolidinetricarboxylato(2-)- κ N1, κ O2](triphenylphosphine)-, (SP-4-3)- (9CI) (CA INDEX NAME)IT 248282-26-0P 248282-27-1P 248282-31-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(ortho-palladated enolates from Schiff bases of amino acid esters as dipoles in [2+3] cycloaddn. reactions)

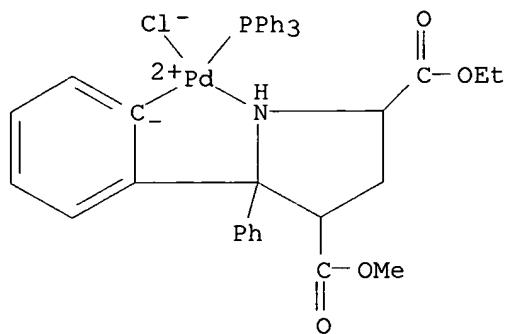
RN 248282-26-0 HCPLUS

CN Palladium, [2-ethyl 4-methyl 2,5-dihydro-5-(phenyl- κ C2)-5-phenyl-1H-pyrrole-2,4-dicarboxylato(2-)- κ N1, κ O2'](triphenylphosphine)-, (SP-4-3)- (9CI) (CA INDEX NAME)



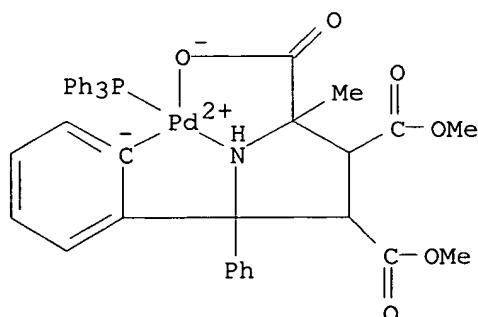
RN 248282-27-1 HCPLUS

CN Palladium, chloro[rel-2-[(1R,2R,3R,5R)-5-(ethoxycarbonyl)-3-(methoxycarbonyl)-2-phenyl-2-pyrrolidinyl- κN]phenyl- κC](triphenylphosphine)-, (SP-4-4)- (9CI) (CA INDEX NAME)



RN 248282-31-7 HCPLUS

CN Palladium, [rel-3,4-dimethyl (1R,2S,3S,4S,5S)-2-methyl-5-(phenyl- $\kappa\text{C}2$)-5-phenyl-2,3,4-pyrrolidinetricarboxylato(2-)- $\kappa\text{N}1,\kappa\text{O}2$](triphenylphosphine)-, (SP-4-3)- (9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 34, 75

IT 248281-95-0P 248281-98-3P 248282-02-2P 248282-09-9P

248282-19-1P 248282-28-2P 248282-30-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP

(Preparation)

(crystal structure; ortho-palladated enolates from Schiff bases of amino acid esters as dipoles in [2+3] cycloaddn. reactions)

IT 248281-97-2P 248282-08-8P **248282-29-3P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP

(Preparation)

(mol. structure; ortho-palladated enolates from Schiff bases of amino acid esters as dipoles in [2+3] cycloaddn. reactions)

IT 248281-87-0P 248281-89-2P 248281-91-6P 248281-93-8P
 248282-00-0P 248282-04-4P 248282-06-6P 248282-12-4P
 248282-14-6P 248282-16-8P 248282-17-9P 248282-20-4P
 248282-21-5P 248282-23-7P 248282-24-8P 248282-25-9P

248282-26-0P 248282-27-1P 248282-31-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(ortho-palladated enolates from Schiff bases of amino acid esters as dipoles in [2+3] cycloaddn. reactions)

REFERENCE COUNT: 128 THERE ARE 128 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 7 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:383202 HCAPLUS

DOCUMENT NUMBER: 127:81593

TITLE: Regioselective synthesis of η^3 -(N-methoxycarbonyl-7-azabicyclo[2.2.1]hepta-2,5-dienyl)- η^5 -(C5Me5)RuCl complexes

AUTHOR(S): Chen, Zhengming; Luo, Lubin; Nolan, Steven P.; Petersen, Jeffrey L.; Trudell, Mark L.

CORPORATE SOURCE: Department of Chemistry, University of New Orleans, New Orleans, LA, 70148, USA

SOURCE: Journal of Organometallic Chemistry (1997), 533(1-2), 25-30

CODEN: JORCAI; ISSN: 0022-328X

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reactions of Cp*Ru(COD)Cl and CpRu(COD)Cl with N-methoxycarbonyl-7-azabicyclo[2.2.1]hepta-2,5-diene derivs. were found to give η^3 -[N(CO2Me)C6H3(2-p-MeC6H4SO2)(6-CO2Me)(5-Me)]CpRuCl and η^3 -[N(CO2Me)-7-azabicyclo[2.2.1]heptadienyl]Cp*RuCl complexes in good yields (54-78%). The coordination reaction was found to take place regioselectively at the least substituted π -bond of the N-methoxycarbonyl-7-azabicyclo[2.2.1]hepta-2,5-diene derivs. The structures of the complexes were determined by 1H and 13C NMR and the structure of η^3 -[N(CO2Me)C6H3(2-p-MeC6H4SO2)(6-CO2Me)(5-Me)]Cp*RuCl was unequivocally established by x-ray crystallog.

IT **191919-97-8P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP

(Preparation)

(preparation and crystal structure of)

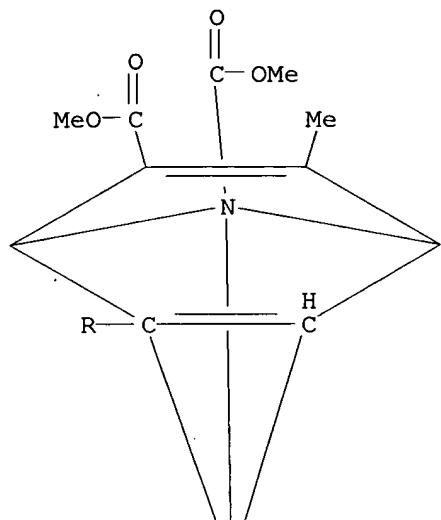
RN 191919-97-8 HCAPLUS

CN Ruthenium, chloro[(5,6- η)-dimethyl 3-methyl-6-[(4-methylphenyl)sulfonyl]-7-azabicyclo[2.2.1]hepta-2,5-diene-2,7-dicarboxylate- κ N7][(1,2,3,4,5- η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, compd. with benzene (2:1) (9CI) (CA INDEX NAME)

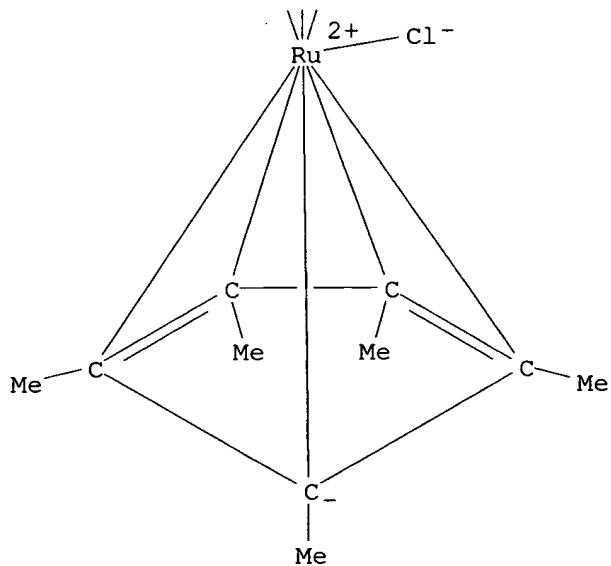
CM 1

CRN 191919-96-7
CMF C28 H34 Cl N O6 Ru S
CCI CCS

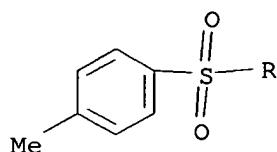
PAGE 1-A



PAGE 2-A



PAGE 3-A



CM 2

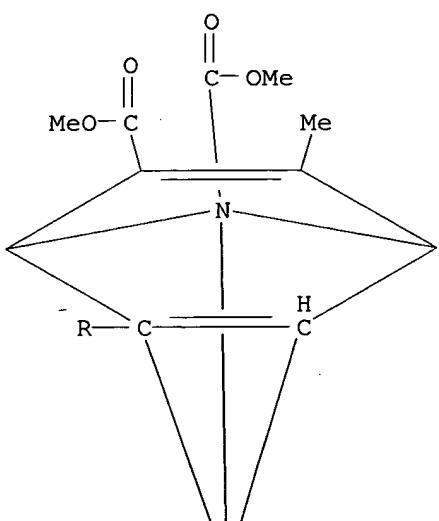
CRN 71-43-2
CMF C6 H6

IT 191919-96-7P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP
 (Preparation)
 (preparation and mol. structure of)

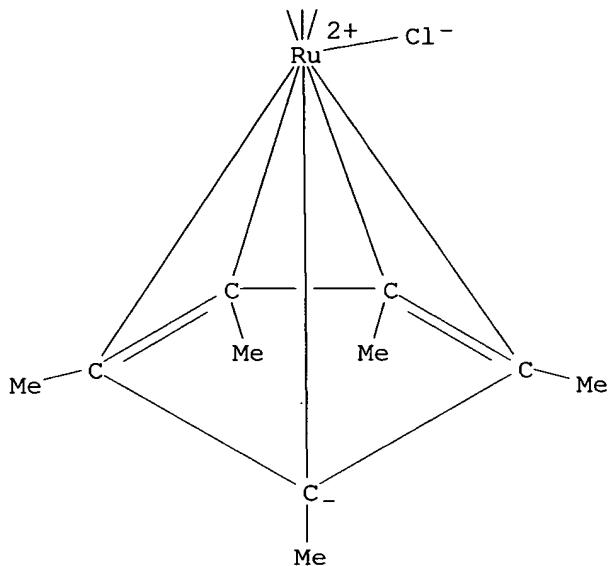
RN 191919-96-7 HCPLUS

CN Ruthenium, chloro[(5,6-η)-dimethyl 3-methyl-6-[(4-methylphenyl)sulfonyl]-7-azabicyclo[2.2.1]hepta-2,5-diene-2,7-dicarboxylate-κN7][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)

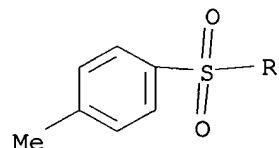
PAGE 1-A



PAGE 2-A



PAGE 3-A



IT 191919-95-6P 191919-98-9P 191919-99-0P

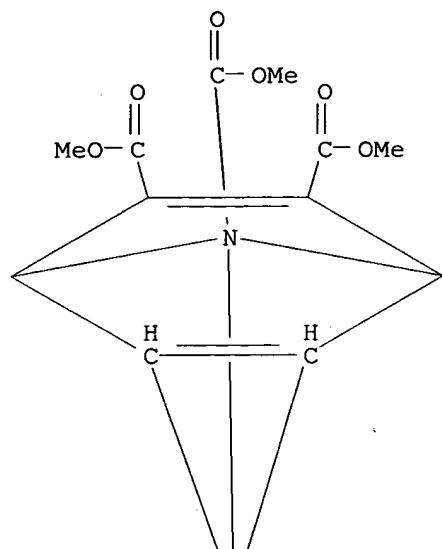
191920-00-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

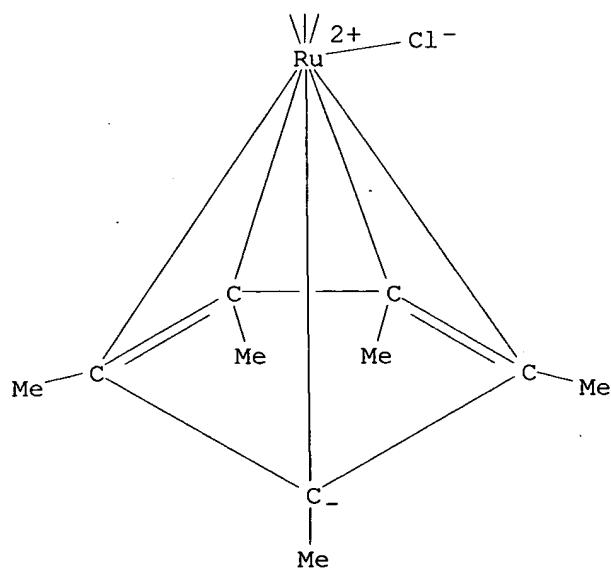
RN 191919-95-6 HCPLUS

CN Ruthenium, chloro[(1,2,3,4,5- η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl][(5,6- η)-trimethyl 7-azabicyclo[2.2.1]hepta-2,5-diene-2,3,7-tricarboxylate- κ N7]- (9CI) (CA INDEX NAME)

PAGE 1-A



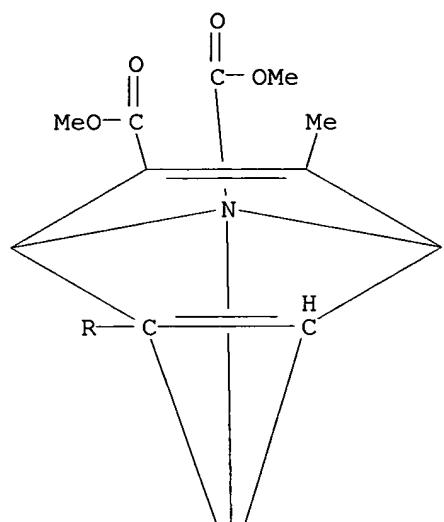
PAGE 2-A



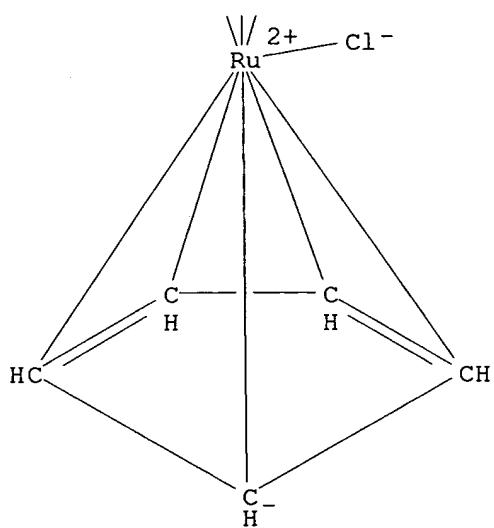
RN 191919-98-9 HCPLUS

CN Ruthenium, chloro(η^5 -2,4-cyclopentadien-1-yl)[(5,6- η)-dimethyl 3-methyl-6-[(4-methylphenyl)sulfonyl]-7-azabicyclo[2.2.1]hepta-2,5-diene-2,7-dicarboxylate- κ N7]- (9CI)
(CA INDEX NAME)

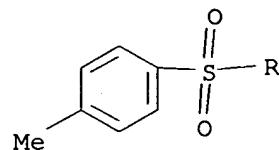
PAGE 1-A



PAGE 2-A



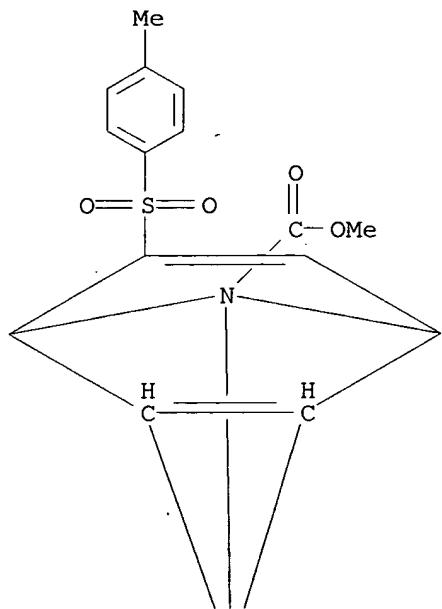
PAGE 3-A



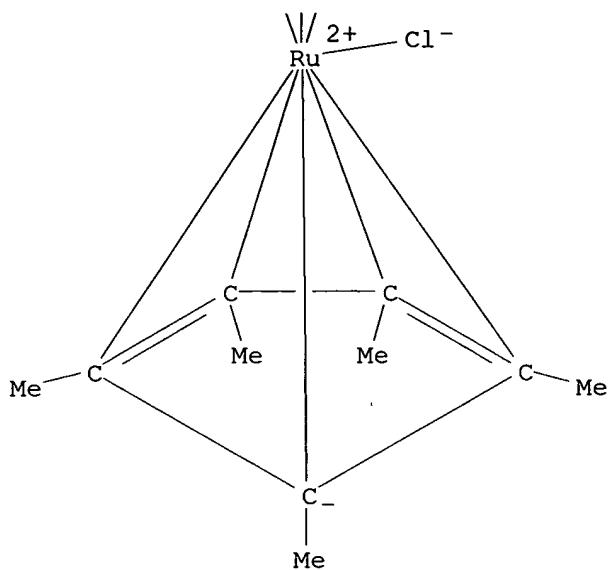
RN 191919-99-0 HCAPLUS

CN Ruthenium, chloro[(5,6- η)-methyl 2-[(4-methylphenyl)sulfonyl]-7-azabicyclo[2.2.1]hepta-2,5-diene-7-carboxylate- κ N7][(1,2,3,4,5- η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



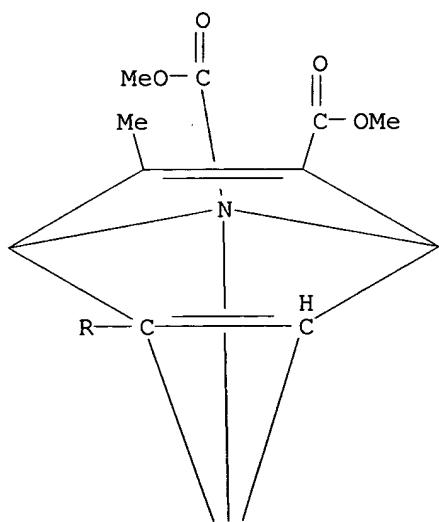
PAGE 2-A



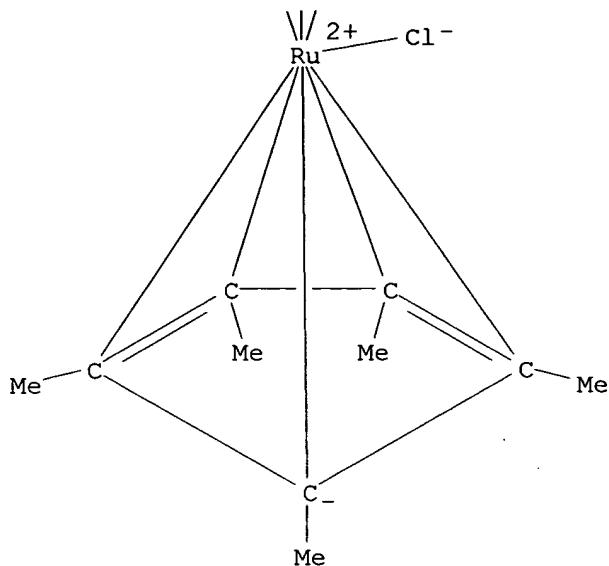
RN 191920-00-0 HCPLUS

CN Ruthenium, chloro[(5,6- η)-dimethyl 3-methyl-5-[(4-methylphenyl)sulfonyl]-7-azabicyclo[2.2.1]hepta-2,5-diene-2,7-dicarboxylate- κ N7][(1,2,3,4,5- η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-(9CI) (CA INDEX NAME)

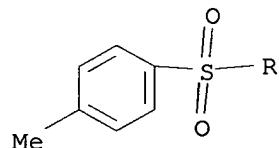
PAGE 1-A



PAGE 2-A



PAGE 3-A



CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75

IT 191919-97-8P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and crystal structure of)

IT 191919-96-7P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and mol. structure of)

IT 191919-95-6P 191919-98-9P 191919-99-0P
 191920-00-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L21 ANSWER 8 OF 17 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:377726 HCPLUS

DOCUMENT NUMBER: 127:17776

TITLE: Comparative Reactivity of Triruthenium and
 Triosmium $\mu_3\text{-}\eta^2\text{-Imidoyls. 2. Reactions}$

with Alkynes

AUTHOR(S): Kabir, Shariff E.; Rosenberg, Edward; Milone, Luciano; Gobetto, Roberto; Osella, Domenico; Rovera, Mauro; McPhillips, Timothy; Day, Michael W.; Carlot, Douglas; Hajela, Sharad; Wolf, Erich; Hardcastle, Kenneth

CORPORATE SOURCE: Department of Chemistry, University of Montana, Missoula, MT, 59812, USA

SOURCE: Organometallics (1997), 16(12), 2674-2681
CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:17776

AB The reactions of $\text{Ru}_3(\text{CO})_9(\mu_3\text{-}\eta_2\text{-CH}_3\text{:NCH}_2\text{CH}_3)(\mu\text{-H})$ (1), $\text{M}_3(\text{CO})_9(\mu_3\text{-}\eta_2\text{-C:N(CH}_2\text{)}_3)(\mu\text{-H})$ ($\text{M} = \text{Ru}$ (2), $\text{M} = \text{Os}$ (3)) with the alkynes RC.tplbond.CR ($\text{R} = \text{CH}_3$, C_6H_5 , CO_2Me) have been studied. The ruthenium complexes 1 and 2 react with 2-butyne at 70° to give two very different trimetallic alkyne derivs.: $\text{Ru}_3(\text{CO})_7(\mu\text{-}\eta_2\text{:}\eta_4\text{-C}_4(\text{CH}_3)_4)(\mu\text{-}\eta_2\text{-CH}_3\text{:NCH}_2\text{CH}_3)(\eta_1\text{-COC(CH}_3\text{)C(H)CH}_3)$ (5) and $\text{Ru}_3(\text{CO})_8(\mu_3\text{-}\eta_2\text{-C:N(CH}_2\text{)}_3)(\mu\text{-}\eta_2\text{-CH}_3\text{C(H):CCH}_3)$ (6). The osmium imidooyl 3 does not react with 2-butyne even at elevated temps. However, the reaction of $\text{Os}_3(\text{CO})_9(\mu\text{-}\eta_2\text{-C:N(CH}_2\text{)}_3)(\mu\text{-H})(\text{CH}_3\text{CN})$ (7b), synthesized from $\text{Os}_3(\text{CO})_{10}(\mu\text{-}\eta_2\text{-C:N(CH}_2\text{)}_3)$ (7a), with 2-butyne yields the analog of 6, $\text{Os}_3(\text{CO})_8(\mu_3\text{-}\eta_2\text{-C:N(CH}_2\text{)}_3)(\mu\text{-}\eta_2\text{-RC(H):CR})$ ($\text{R} = \text{CH}_3$ (10), $\text{R} = \text{C}_6\text{H}_5$ (11)) on thermolysis of the initially formed nonacarbonyl precursors (8 and 9 for $\text{R} = \text{CH}_3$), which are a mixture of isomers. Direct reaction of 7a with diphenylacetylene at 100° gives somewhat lower yields of 11. The reaction of 7b with di-Me acetylenedicarboxylate or the direct reaction of 3 with this alkyne yields the nonacarbonyl derivative $\text{Os}_3(\text{CO})_9(\mu\text{-}\eta_2\text{-C:N(CH}_2\text{)}_3)(\mu_3\text{-}\eta_3\text{-CH}_3\text{O}_2\text{CC:C(H)CO}_2\text{CH}_3)$ (12). Direct reaction of 7a with a 2.5 M excess trimethylamine N-oxide at room temperature yields the alkyne-imidooyl-coupled product $\text{Os}_3(\text{CO})_8(\mu\text{-}\eta_6\text{-CH}_3\text{C(H):C(CH}_3\text{)C(CH}_3\text{):C(CH}_3\text{)C:N(CH}_2\text{)}_3)$ (13). The solid state structures of 5, 11, 12, and 13 are reported. A comparative study of the electrochem. properties of 5 and 1 is also reported.

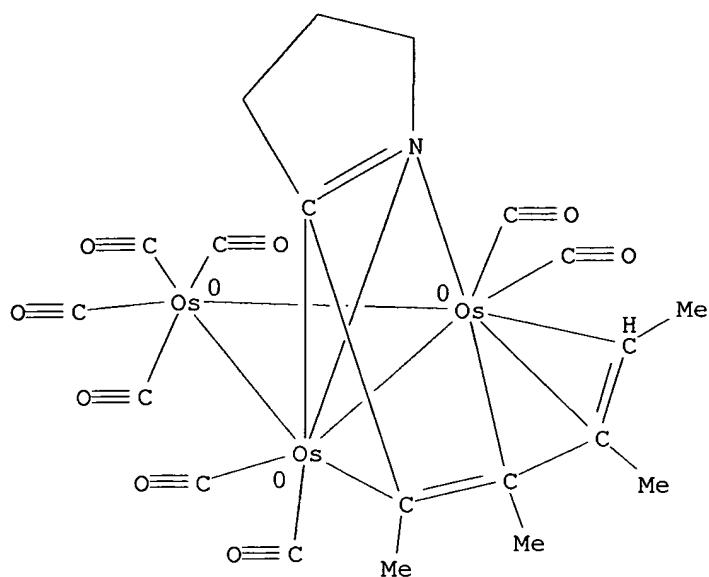
IT 190451-99-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and crystal structure of)

RN 190451-99-1 HCAPLUS

CN Osmium, octacarbonyl[μ -[$\eta_3\text{:}\eta_3$ -3,4-dihydro-5-(1,2,3-trimethyl-1,3-pentadienyl)-2H-pyrrole- κN]]tri-, triangulo, stereoisomer (9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 72, 75

IT 190451-94-6P 190451-97-9P **190451-99-1P**
 RL: PRP (Properties); SPN (Synthetic preparation); PREP
 (Preparation)

(preparation and crystal structure of)

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L21 ANSWER 9 OF 17 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:400976 HCPLUS

DOCUMENT NUMBER: 125:276164

TITLE: Synthesis and spectral studies of 1,3-diketonate
 derivatives of ortho-palladated
 α -arylalkylamines

AUTHOR(S): Dunina, V. V.; Zalevskaya, O. A.; Palii, S. P.;
 Zagorevskii, D. V.; Nekrasov, Yu. S.

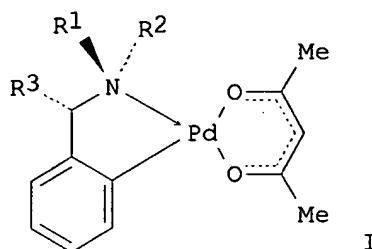
CORPORATE SOURCE: Khimicheskii Fakul'tet, Moskovskii
 Gosudarstvennyi Universitet im. M. V.
 Lomonosova, Moscow, 119899, Russia

SOURCE: Izvestiya Akademii Nauk, Seriya Khimicheskaya
 (1996), (3), 733-740

CODEN: IASKEA
 PUBLISHER: Institut Organicheskoi Khimii im. N. D.

Zelinskogo Rossiiskoi Akademii Nauk
 LANGUAGE: Journal
 Russian

GI



AB Acetylacetonate derivs. of a series of ortho-palladated secondary and tertiary α -aryl-alkylamines (e.g., I; R₁ = R₂ = R₃ = Me; R₁, R₂ = H, Pri, R₃ = Me) were prepared; their structure and stereochem. were elucidated by IR, UV, ¹H NMR and CD spectra. The fragmentation processes of these complexes and some model compds. were investigated by EI mass spectrometry. An unusual rearrangement involving migration of hydrogen atom from an alkylaminoalkyl group to a palladium atom leading to a hydride intermediate and followed by PdH elimination was observed. The rearrangement was assumed to occur through isomerization of η^2 -O,O'-coordinated β -diketonate ligand into the η^1 -C-bonded diketonyl form to give coordinative unsatd. metal center.

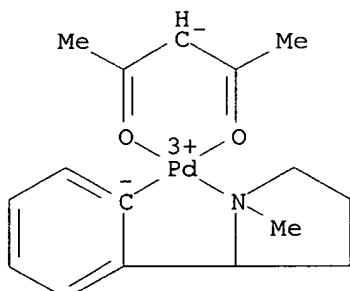
IT 150950-20-2

RL: PRP (Properties)

(synthesis and spectra of diketonate derivs. of ortho-palladated α -arylalkylamines)

RN 150950-20-2 HCPLUS

CN Palladium, [2-(1-methyl-2-pyrrolidinyl)phenyl-C,N] (2,4-pentanedionato-O,O')-, (SP-4-3)- (9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 73

IT 150950-20-2 169518-54-1

RL: PRP (Properties)

(synthesis and spectra of diketonate derivs. of ortho-palladated α -arylalkylamines)

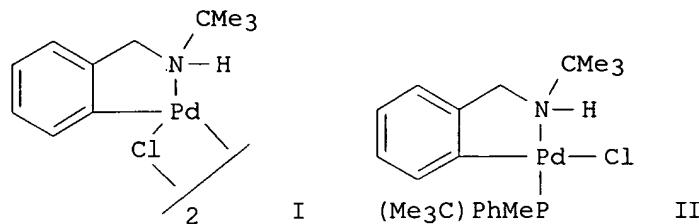
L21 ANSWER 10 OF 17 HCPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:991292 HCPLUS

DOCUMENT NUMBER: 124:261280

TITLE: Enantiomeric discrimination in the complexation of ortho-palladated α -arylalkylamines with the racemic tert-butylmethylphenylphosphine

AUTHOR(S): Dunina, V. V.; Golovan, E. B.; Gulyukina, N. S.;
Buyevich, A. V.
CORPORATE SOURCE: Dept. Chem., M. V. Lomonosov Moscow State Univ.,
Moscow, 119899, Russia
SOURCE: Tetrahedron: Asymmetry (1995), 6(11), 2731-46
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:261280
GI



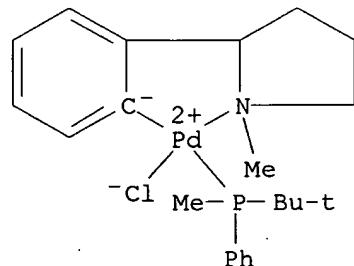
AB A high degree of diastereoselectivity was achieved in the coordination of monodentate phosphine PMeButPh with dimeric chloro-bridged ortho-palladated complexes in solution due to the modification of the stereoselective structure, by the creation of asymmetry in the environment of N donor atom and by the fitting of substituents sizes in the palladacycle. For example, racemic I reacts with racemic PMeButPh to give II with diastereoselectivity > 10:1. The stereochem. of complexation is discussed in the terms of equilibrium consts. between two diastereomers of monophosphine complexes from the ^{31}P NMR data.

IT 174388-64-8P

RL: BYP (Byproduct); PREP (Preparation)
(enantiomeric discrimination in complexation of ortho-palladated
 α -arylalkylamines with racemic tert-
butylmethylphenylphosphine)

RN 174388-64-8 HCAPLUS

CN Palladium, chloro[(1,1-dimethylethyl)methylphenylphosphine][2-(1-methyl-2-pyrrolidinyl)phenyl-C,N]-, [SP-4-4-2(S),3(1R-cis)]- (9CI) (CA INDEX NAME)

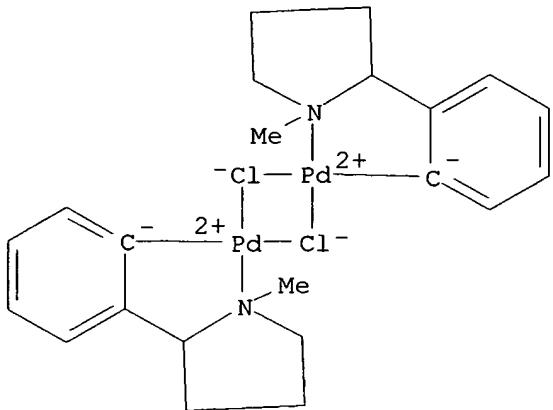


IT 175273-20-8
RL: RCT (Reactant); RACT (Reactant or reagent)

(enantiomeric discrimination in complexation of ortho-palladated α -arylalkylamines with racemic tert-butylmethylphenylphosphine)

RN 175273-20-8 HCAPLUS

CN Palladium, di- μ -chlorobis[2-(1-methyl-2-pyrrolidinyl- κ N)phenyl- κ C]di-, stereoisomer (9CI) (CA INDEX NAME)

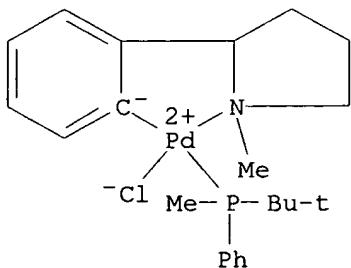


IT 173914-32-4P 174061-26-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(enantiomeric discrimination in complexation of ortho-palladated α -arylalkylamines with racemic tert-butylmethylphenylphosphine)

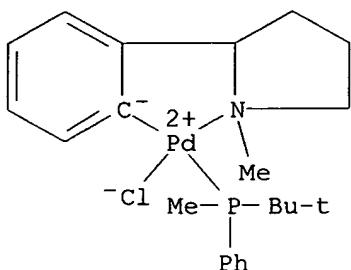
RN 173914-32-4 HCAPLUS

CN Palladium, chloro[(1,1-dimethylethyl)methylphenylphosphine][2-(1-methyl-2-pyrrolidinyl)phenyl-C,N]-, [SP-4-4-2(R),3(1R-cis)]- (9CI) (CA INDEX NAME)



RN 174061-26-8 HCAPLUS

CN Palladium, chloro[(1,1-dimethylethyl)methylphenylphosphine][2-(1-methyl-2-pyrrolidinyl)phenyl-C,N]-, [SP-4-4-(cis)]- (9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 68

IT 64998-29-4P 147021-30-5P 147126-34-9P 147126-36-1P
147126-37-2P 147126-38-3P 174061-27-9P 174061-28-0P

174388-64-8P

RL: BYP (Byproduct); PREP (Preparation)

(enantiomeric discrimination in complexation of ortho-palladated α -arylalkylamines with racemic tert-butylmethylphenylphosphine)

IT 7621-16-1, tert-Butyl(methyl)(phenyl)phosphine 34424-15-2
73089-54-0 90581-44-5 92999-94-5 135637-49-9 150576-36-6
173914-26-6 174061-13-3 174061-15-5 174061-16-6 174061-17-7
174061-18-8 174061-20-2 174061-21-3 **175273-20-8**

RL: RCT (Reactant); RACT (Reactant or reagent)

(enantiomeric discrimination in complexation of ortho-palladated α -arylalkylamines with racemic tert-butylmethylphenylphosphine)

IT 64867-66-9P 147021-29-2P 147021-31-6P 147021-32-7P
147126-35-0P 147126-39-4P 173914-27-7P 173914-28-8P
173914-29-9P 173914-30-2P 173914-31-3P **173914-32-4P**
174061-22-4P 174061-23-5P 174061-24-6P 174061-25-7P

174061-26-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(enantiomeric discrimination in complexation of ortho-palladated α -arylalkylamines with racemic tert-butylmethylphenylphosphine)

L21 ANSWER 11 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:650135 HCAPLUS

DOCUMENT NUMBER: 119:250135

TITLE: Chiral cyclopalladated complexes based on 1-methyl-2-phenylpyrrolidine

AUTHOR(S): Dunina, V. V.; Kisliv, V. P.; Gulyukina, N. S.; Grishin, Yu. K.; Beletskaya, I. P.

CORPORATE SOURCE: Mosk. Gos. Univ., Moscow, Russia

SOURCE: Metalloorganicheskaya Khimiya (1992), 5(6), 1297-305

CODEN: MEKHEX; ISSN: 0235-0114

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 119:250135

AB Cyclopalladated complex di- μ -chlorobis(1-methyl-2-phenylpyrrolidinato-2'C,N)dipalladium(II) with a configurationally fixed asym. donor nitrogen atom was obtained in a high yield by direct cyclopalladation of 1-methyl-2-phenylpyrrolidine. Structures of both the dimeric complex and its mononuclear derivs. were

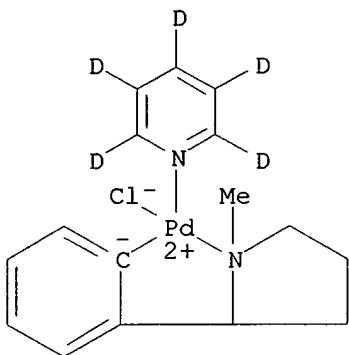
established by UV, IR, 1H NMR and mass spectroscopy. The racemic dimer complex was resolved via its (S)-prolinate complexes.

IT 150938-98-0P

RL: PREP (Preparation)
(formation and proton NMR of)

RN 150938-98-0 HCPLUS

CN Palladium, chloro[2-(1-methyl-2-pyrrolidinyl)phenyl- κ N] (pyridine-d5)-, (SP-4-4)- (9CI) (CA INDEX NAME)

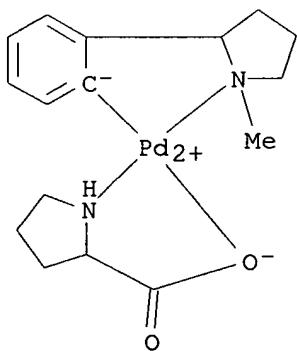


IT 150952-81-1P 151062-05-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation and reaction of, with hydrochloric acid)

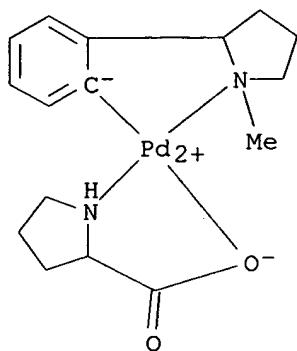
RN 150952-81-1 HCPLUS

CN Palladium, [2-[(1S,2S)-1-methyl-2-pyrrolidinyl- κ N]phenyl- κ C][(1R)-L-prolinato- κ N1, κ O2]-, (SP-4-4)- (9CI)
(CA INDEX NAME)



RN 151062-05-4 HCPLUS

CN Palladium, [2-[(1S,2S)-1-methyl-2-pyrrolidinyl- κ N]phenyl- κ C][(1S)-L-prolinato- κ N1, κ O2]-, (SP-4-4)- (9CI)
(CA INDEX NAME)

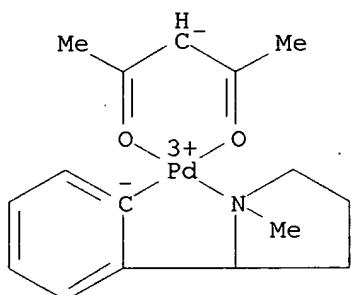


IT 150950-20-2B

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 150950-20-2 HCPLUS

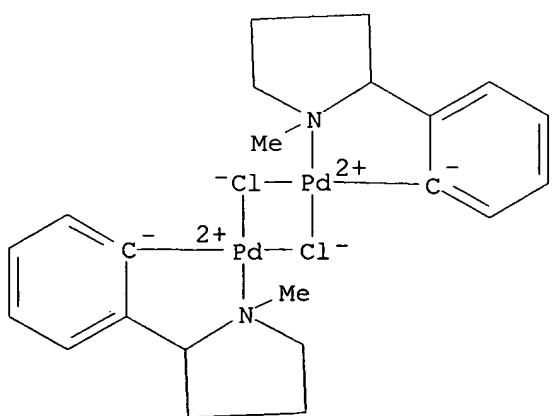
CN Palladium, [2-(1-methyl-2-pyrrolidinyl)phenyl-C,N](2,4-pentanedionato-O,O')-, (SP-4-3)- (9CI) (CA INDEX NAME)



IT 139048-42-3B

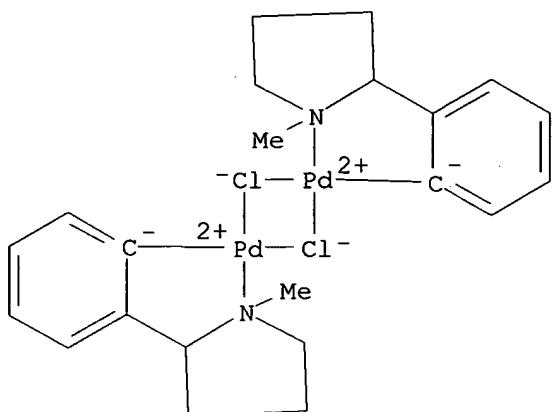
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, resolution, and reaction of racemic, with potassium acetylacetone, and CD spectra of resolved isomers)

RN 139048-42-3 HCPLUS

CN Palladium, di- μ -chlorobis[2-(1-methyl-2-pyrrolidinyl)phenyl-C,N]di- (9CI) (CA INDEX NAME)

CC 29-13 (Organometallic and Organometalloidal Compounds)
IT **150938-98-0P**
RL: PREP (Preparation)
(formation and proton NMR of)
IT **150952-81-1P 151062-05-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation and reaction of, with hydrochloric acid)
IT **150950-20-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **139048-42-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, resolution, and reaction of racemic, with potassium
acetylacetone, and CD spectra of resolved isomers)

L21 ANSWER 12 OF 17 HCPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:243701 HCPLUS
DOCUMENT NUMBER: 116:243701
TITLE: A comparison of the electrochemical properties
of cyclopalladated compounds and the
corresponding coordination complexes without
metal-carbon bonds
AUTHOR(S): Butin, K. P.; Rakhimov, R. D.; Gulyukina, N. S.;
Dunina, V. V.; Beletskaya, I. P.
CORPORATE SOURCE: Mosk. Gos. Univ., Moscow, USSR
SOURCE: Metalloorganicheskaya Khimiya (1991), 4(6),
1293-302
CODEN: MEKHEX; ISSN: 0235-0114
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Oxidation (EOx) and reduction (ERed) potentials of a series of the
cyclopalladated compds. were measured by cyclic and linear
voltammetry on a Pt electrode. The compds. were prepared from
secondary and tertiary α -arylalkylamines as well as from
several coordination bis-complexes of palladium(II) chloride with
secondary α -arylalkylamines having no σ -bonds C-Pd and
the corresponding amine ligands (EOx only). The readiness of oxidation
decreases in the order: free amines > cyclopalladated compds. >
coordination complexes. The tendency to reduction decreases in the
reverse order. The results are interpreted with the help of the
qual. MO theory in the terms «reduction at metal»,
«oxidation at ligand» et al. Possible mechanisms of the
electrode reactions are discussed.
IT **139048-42-3**
RL: PRP (Properties)
(oxidation and reduction potential of)
RN 139048-42-3 HCPLUS
CN Palladium, di- μ -chlorobis[2-(1-methyl-2-pyrrolidinyl)phenyl-
C,N]di- (9CI) (CA INDEX NAME)



CC 72-2 (Electrochemistry)

Section cross-reference(s): 29, 78

IT 103-83-3 938-36-3 3378-72-1 4151-44-4 17279-31-1
 18987-59-2 19302-32-0 51371-44-9 64822-34-0 69187-61-7
 85737-43-5 85737-44-6 92973-56-3 104111-85-5 104111-88-8
 105120-16-9 106224-62-8 106402-45-3 139048-36-5 139048-37-6
139048-42-3 139048-43-4 139163-80-7 140851-27-0

RL: PRP (Properties)

(oxidation and reduction potential of)

L21 ANSWER 13 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:151973 HCAPLUS

DOCUMENT NUMBER: 116:151973

TITLE: Synthesis, structure and adsorption behavior of a new palladium bipyrrrole complex

AUTHOR(S): Gao, Yang; Su, Feng; Liu, Shangchang; Wu, Linyou; Yu, Baoqiang; Zhang, Deqi

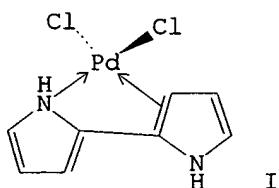
CORPORATE SOURCE: Dep. Chem., Liaoning Univ., Shenyang, 110036, Peop. Rep. China

SOURCE: Huaxue Xuebao (1991), 49(12), 1450-6
CODEN: HHHPA4; ISSN: 0567-7351

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

GI



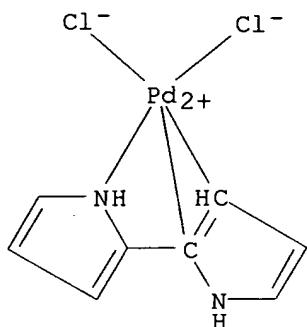
AB Studies on the preparation and structure of palladium dichloride bipyrrrole complex I and its adsorption behavior with H2 are reported. The mechanism of H2 adsorption are discussed. Theor. calcns. (CNDO/2) are in good agreement with exptl. results.

IT **139604-58-3**

RL: PRP (Properties)

(MO calcns. of, tetrahedral structure vs.)

RN 139604-58-3 HCAPLUS
 CN Palladium, [(2,3- η)-2,2'-bi-1H-pyrrole-N']dichloro- (9CI) (CA
 INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 66

IT 139604-57-2 139604-58-3

RL: PRP (Properties)

(MO calcns. of, tetrahedral structure vs.)

L21 ANSWER 14 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:406718 HCAPLUS

DOCUMENT NUMBER: 109:6718

TITLE: Rupture and repair of the porphyrin inner core:
carbon-nitrogen bond breaking and formation in
ruthenium complexes of an N,N'-bridged porphyrinAUTHOR(S): Balch, Alan L.; Chan, Yee Wai; Olmstead, Marilyn
M.; Renner, Mark W.; Wood, Fred E.CORPORATE SOURCE: Dep. Chem., Univ. California, Davis, CA, 95616,
USASOURCE: Journal of the American Chemical Society (1988),
110(12), 3897-902

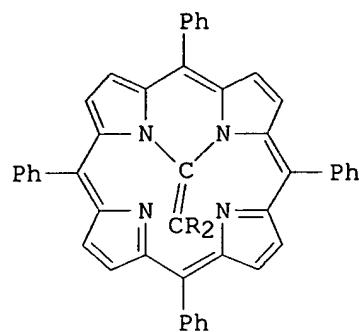
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

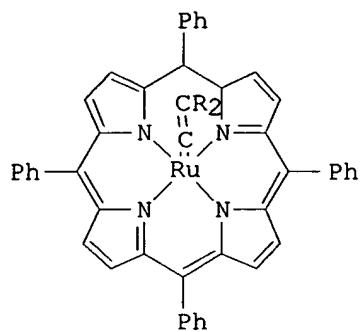
LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:6718

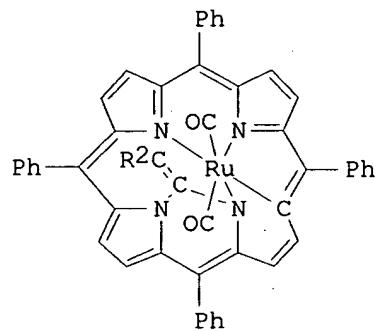
GI



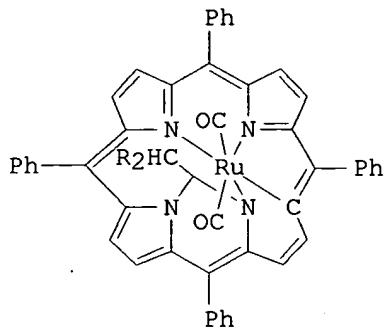
I



II



III



IV

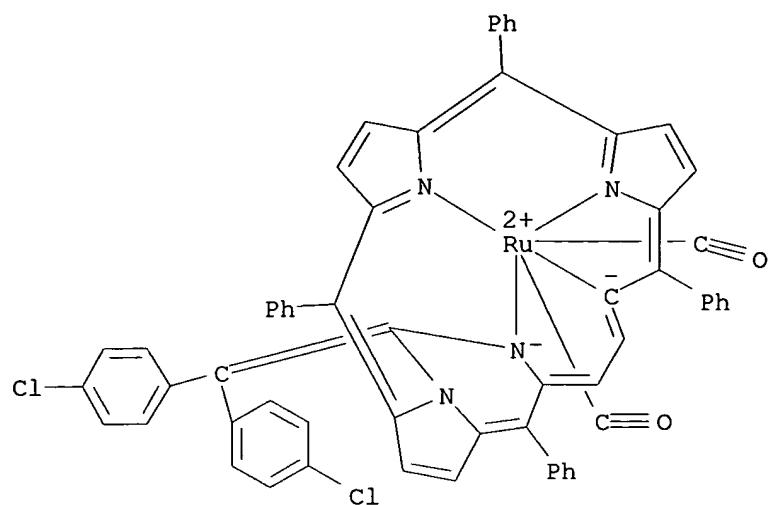
AB Treatment of the N,N'-vinyl-bridged porphyrin I ($R = C_6H_4Cl-p$) with $Ru_3(CO)_{12}$ yields three products: the carbene complex II and two $Ru(II)$ dicarbonyl complexes III and IV in which the N,N'-bridge remains intact, but the Ru has inserted into a pyrrole C-N bond. The crystal structure of IV was determined. The Ru is six-coordinate with two cis CO ligands, bonds to two normal pyrrole groups, and bonds to the C and N of the ring-opened pyrrole. The damaged porphyrin is no longer planar. Upon heating, both III and IV undergo C-N bond formation to reform the porphyrin ring.

IT 90194-59-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 90194-59-5 HCAPLUS

CN Ruthenium, [1-[bis(4-chlorophenyl)methylene]-1,2-dihydro-7,12,17,22-tetraphenyl-3,20-metheno-8,11:13,16-dinitrilo-11H-pyrrolo[1,2-c][1,3]diazacyclononadecinato(2-)C6,N2,N23,N24]dicarbonyl-, (OC-6-45)- (9CI) (CA INDEX NAME)



IT 114299-72-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal and mol. structure of)

RN 114299-72-8 HCPLUS

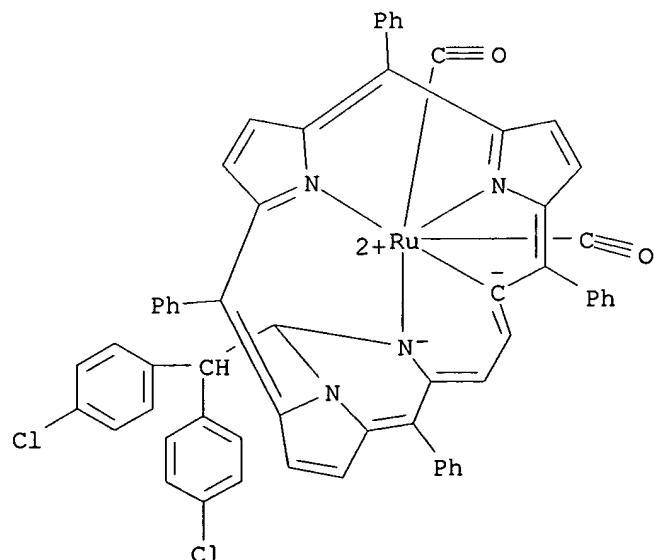
CN Ruthenium, [1-[bis(4-chlorophenyl)methyl]-1,2-dihydro-7,12,17,22-tetraphenyl-3,20-metheno-8,11:13,16-dinitriolo-11H-pyrrolo[1,2-c][1,3]diazacyclononadecinato(2-)C6,N2,N23,N24]dicarbonyl-,
(OC-6-45)-, compd. with dichloromethane (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 114299-71-7

CMF C60 H38 Cl2 N4 O2 Ru

CCI CCS



CM 2

CRN 75-09-2
CMF C H2 Cl2Cl-CH₂-ClCC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 26, 75IT 87532-89-6P 90194-59-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)IT 114299-72-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal and mol. structure of)

L21 ANSWER 15 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:591369 HCAPLUS

DOCUMENT NUMBER: 105:191369

TITLE: Ortho-palladated imines as precursors of
metallo-1,3-dipoles

AUTHOR(S): Grigg, Ronald; Devlin, John

CORPORATE SOURCE: Chem. Dep., Queen's Univ., Belfast, BT9 5AG, UK

SOURCE: Journal of the Chemical Society, Chemical
Communications (1986), (8), 631-2

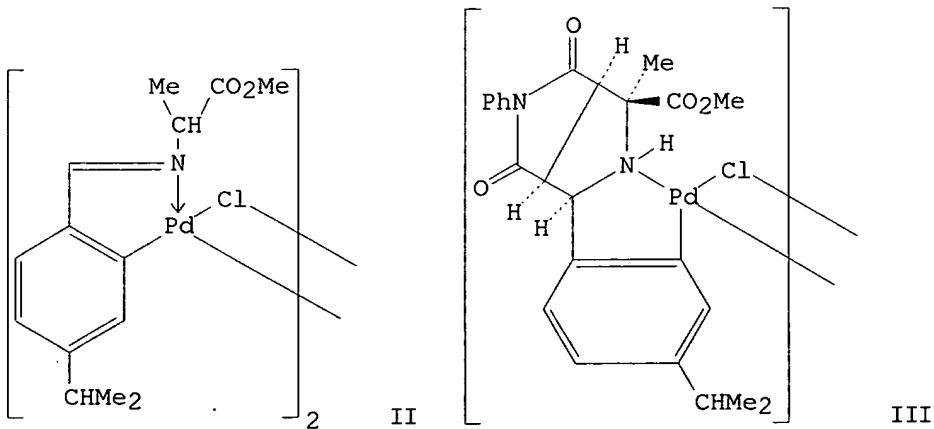
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 105:191369

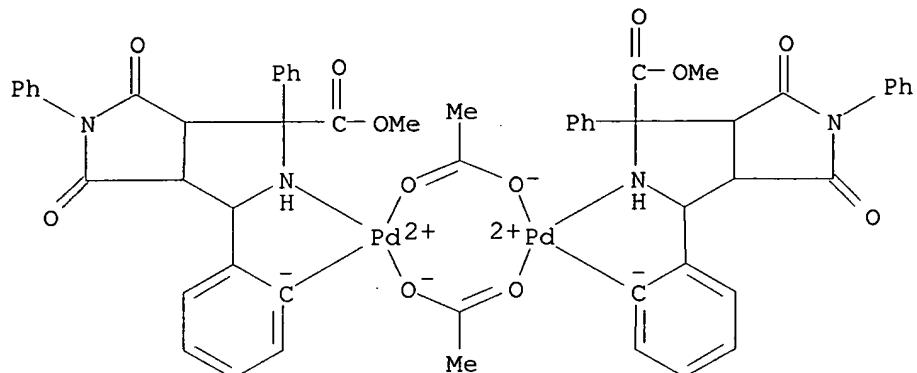
GI

AB Deprotonation of ortho palladated imines of α -amino acid esters by Et₃N at room temperature gave metallo-1,3-dipoles which were trapped by cycloaddn. to N-phenylmaleimide (I). Treatment of 4-Me₂CHC₆H₄CH:NCHMeCO₂Me with LiPdCl₄ in MeOH gave 84% palladated imine II which was deprotonated by Et₃N in CH₂Cl₂ containing I to give 84% cycloadduct III.

IT 105117-62-2P

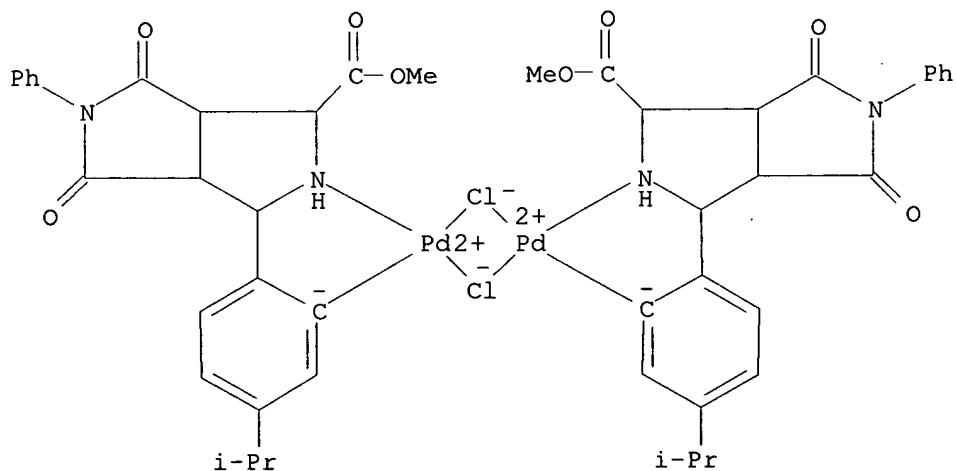
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (preparation and reaction of, with picoline)

RN 105117-62-2 HCPLUS
 CN Palladium, bis[μ -(acetato-O:O')]bis[2-[octahydro-3-(methoxycarbonyl)-4,6-dioxo-3,5-diphenylpyrrolo[3,4-c]pyrrol-1-yl]phenyl]di-, stereoisomer (9CI) (CA INDEX NAME)

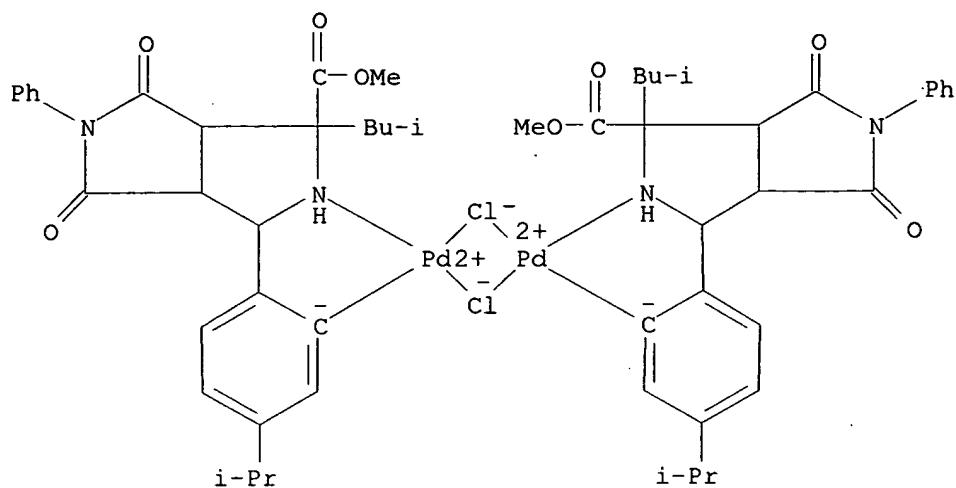


IT 105101-78-8P 105101-79-9P 105101-80-2P
 105101-81-3P 105101-89-1P 105101-90-4P
 105101-91-5P 105117-61-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

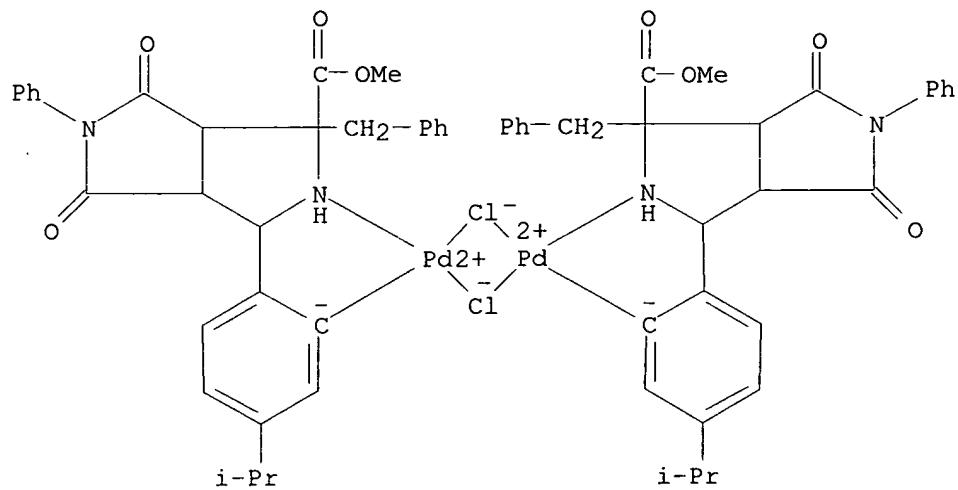
RN 105101-78-8 HCPLUS
 CN Palladium, di- μ -chlorobis[5-(1-methylethyl)-2-[octahydro-3-(methoxycarbonyl)-4,6-dioxo-5-phenylpyrrolo[3,4-c]pyrrol-1-yl]phenyl]di-, stereoisomer (9CI) (CA INDEX NAME)



RN 105101-79-9 HCPLUS
 CN Palladium, di- μ -chlorobis[5-(1-methylethyl)-2-[octahydro-3-(methoxycarbonyl)-3-(2-methylpropyl)-4,6-dioxo-5-phenylpyrrolo[3,4-c]pyrrol-1-yl]phenyl]di-, stereoisomer (9CI) (CA INDEX NAME)

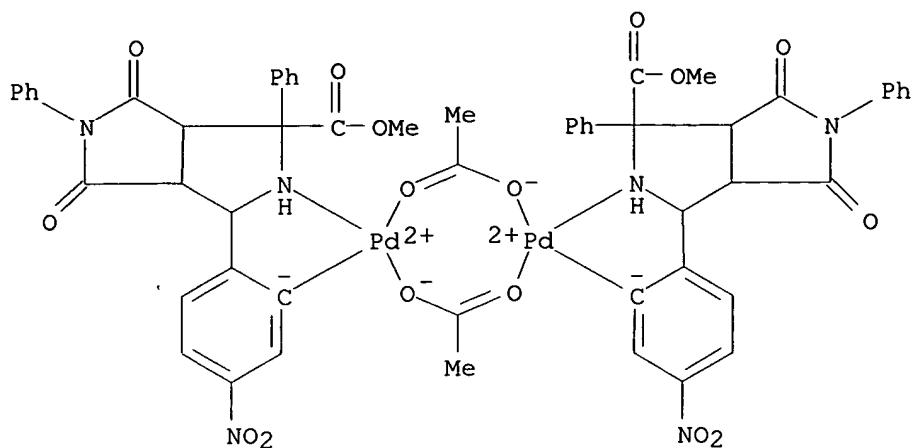


RN 105101-80-2 HCPLUS

CN Palladium, di- μ -chlorobis[5-(1-methylethyl)-2-(methoxycarbonyl)-4,6-dioxo-5-phenyl-1-(phenylmethyl)pyrrolo[3,4-c]pyrrol-1-ylphenyl]di-, stereoisomer (9CI) (CA INDEX NAME)

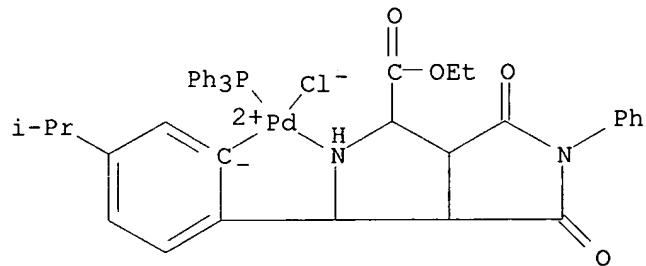
RN 105101-81-3 HCPLUS

CN Palladium, bis[μ -(acetato-O:O')]bis[5-nitro-2-(methoxycarbonyl)-4,6-dioxo-3,5-diphenylpyrrolo[3,4-c]pyrrol-1-ylphenyl]di-, stereoisomer (9CI) (CA INDEX NAME)



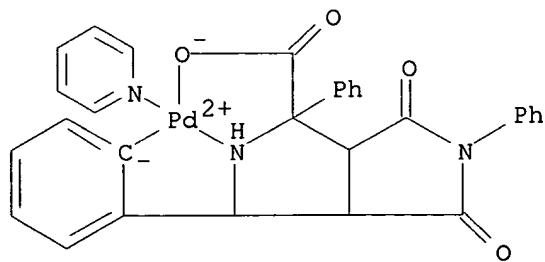
RN 105101-89-1 HCAPLUS

CN Palladium, chloro[2-[3-(ethoxycarbonyl)octahydro-4,6-dioxo-5-phenylpyrrolo[3,4-c]pyrrol-1-yl]-5-(1-methylethyl)phenyl](triphenylphosphine)-, stereoisomer (9CI) (CA INDEX NAME)



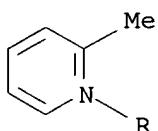
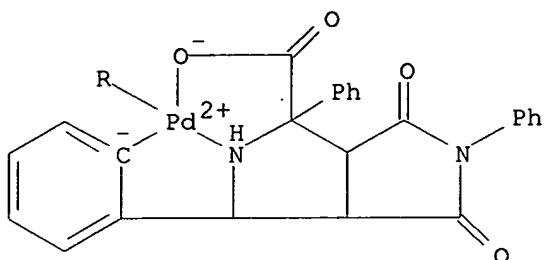
RN 105101-90-4 HCAPLUS

CN Palladium, [octahydro-4,6-dioxo-1,3,5-triphenylpyrrolo[3,4-c]pyrrole-1-carboxylato(2-)](pyridine)-, [SP-4-4-(1α,2α,3α,3β,6αβ)]- (9CI) (CA INDEX NAME)

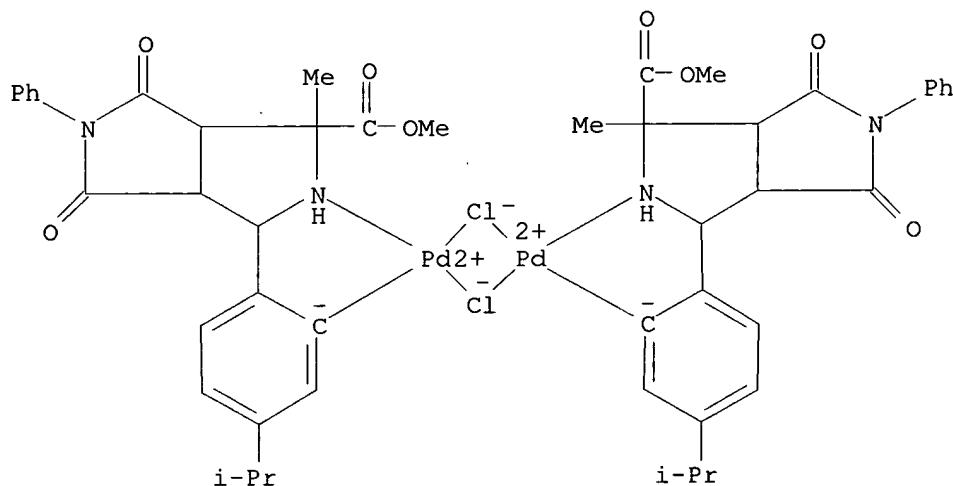


RN 105101-91-5 HCAPLUS

CN Palladium, (2-methylpyridine)[octahydro-4,6-dioxo-1,3,5-triphenylpyrrolo[3,4-c]pyrrole-1-carboxylato(2-)]-, [SP-4-4-(1α,2α,3α,3β,6αβ)]- (9CI) (CA INDEX NAME)



RN 105117-61-1 HCPLUS

CN Palladium, di- μ -chlorobis[5-(1-methylethyl)-2-[octahydro-3-(methoxycarbonyl)-3-methyl-4,6-dioxo-5-phenylpyrrolo[3,4-c]pyrrol-1-yl]phenyl]di-, stereoisomer (9CI) (CA INDEX NAME)CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 34

IT 105117-62-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation and reaction of, with picoline)IT 105086-55-3P 105101-71-1P 105101-75-5P 105101-78-8P
105101-79-9P 105101-80-2P 105101-81-3P

105101-88-0P 105101-89-1P 105101-90-4P

105101-91-5P 105117-61-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)L21 ANSWER 16 OF 17 HCPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:407412 HCPLUS

DOCUMENT NUMBER: 101:7412
TITLE: Remarkable disruption of a porphyrin. Insertion
of a ruthenium atom into a pyrrole
carbon-nitrogen bond of an N,N'-vinyl-bridged
porphyrin
AUTHOR(S): Chan, Yee Wai; Wood, Fred E.; Renner, Mark W.;
Hope, Hakon; Balch, Alan L.
CORPORATE SOURCE: Dep. Chem., Univ. California, Davis, CA, 95616,
USA
SOURCE: Journal of the American Chemical Society (1984),
106(11), 3380-1
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The N,N'-bridged porphyrin I (R = C₆H₄Cl-4) reacted with Ru₃(CO)₁₂ with rupture of a pyrrole C-N bond to give the Ru complex II. The x-ray crystal structure of II showed that the two CO's were cis and the disrupted porphyrin ring was no longer planar, occupying 1 axial and 3 equatorial sites of the approx. octahedral Ru.

IT 90194-60-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP
(Preparation)

(preparation and crystal structure of)

RN 90194-60-8 HCPLUS

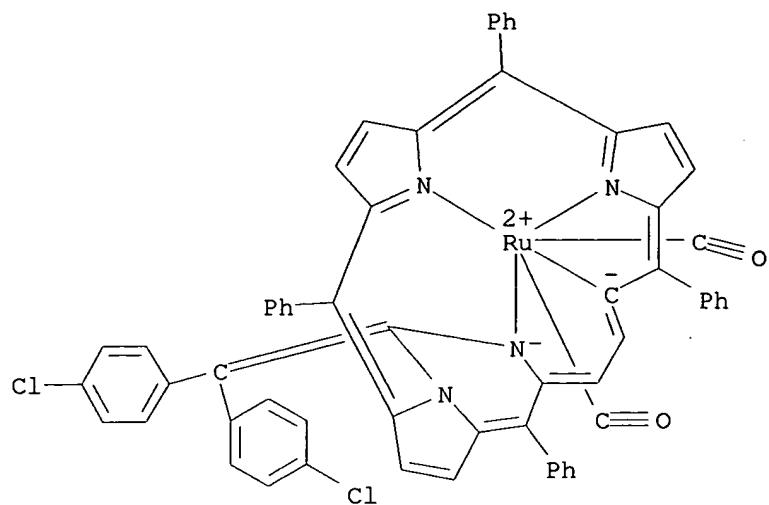
CN Ruthenium, [1-[bis(4-chlorophenyl)methylene]-1,2-dihydro-7,12,17,22-tetraphenyl-3,20-metheno-8,11:13,16-dinitrilo-11H-pyrrolo[1,2-c][1,3]diazacyclononadecinato(2-)C₆,N₂,N₂₃,N₂₄]dicarbonyl-, (OC-6-45)-, compd. with dichloromethane (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 90194-59-5

CMF C₆₀ H₃₆ C₁₂ N₄ O₂ Ru

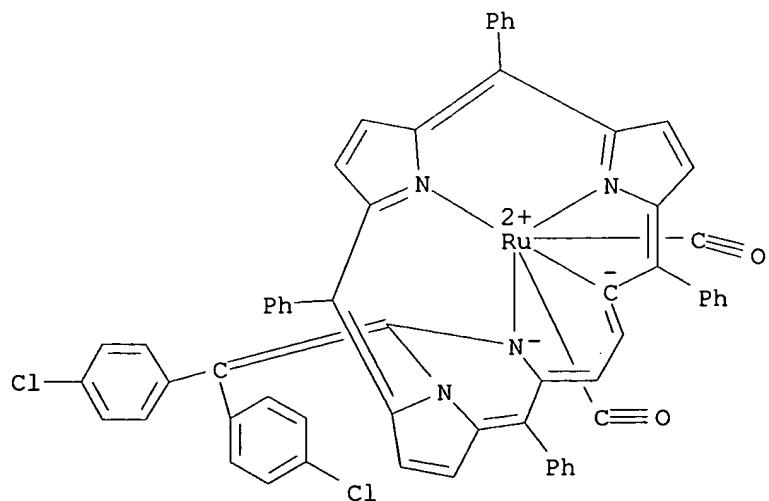
CCI CCS



CM 2

CRN 75-09-2
CMF C H2 Cl2Cl-CH₂-ClIT **90194-59-5P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP
(Preparation)
(preparation and mol. structure of)

RN 90194-59-5 HCPLUS

CN Ruthenium, [1-[bis(4-chlorophenyl)methylene]-1,2-dihydro-7,12,17,22-tetraphenyl-3,20-metheno-8,11:13,16-dinitriolo-11H-pyrrolo[1,2-c][1,3]diazacyclononadecinato(2-)C6,N2,N23,N24]dicarbonyl-,
(OC-6-45)- (9CI) (CA INDEX NAME)

CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 26, 75
 IT **90194-60-8P**
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and crystal structure of)
 IT **90194-59-5P**
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and mol. structure of)

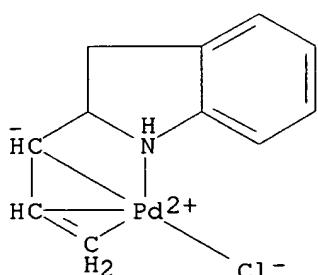
L21 ANSWER 17 OF 17 HCPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1981:406963 HCPLUS
 DOCUMENT NUMBER: 95:6963
 TITLE: Palladium-assisted N-alkylation of indoles:
 attempted application to polycyclization
 AUTHOR(S): Hegedus, Louis S.; Winton, Peter M.; Varaprath,
 Sudarsanan
 CORPORATE SOURCE: Dep. Chem., Colorado State Univ., Fort Collins,
 CO, 80523, USA
 SOURCE: Journal of Organic Chemistry (1981), 46(11),
 2215-21
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 95:6963

AB The palladium(II) complexes of the olefins ethene, propene, and 1-hexene reacted with 1-lithioindole to produce N-alkylated indoles exclusively. Attempts to perform this N-alkylation intramol. (to form tricyclic material from 2-allylindole) failed. Anilines with dienic side chains in the 2-position were subjected to Pd(II)-assisted cyclization conditions in attempts to induce polycyclization. However, only monocyclization was observed

IT **76927-69-0P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 76927-69-0 HCPLUS

CN Palladium, chloro[(1,2,3- η)-1-(2,3-dihydro-1H-indol-2-yl)-2-propenyl]- (9CI) (CA INDEX NAME)



CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
 IT 1557-08-0P 1613-32-7P 1859-90-1P 6639-06-1P 10604-59-8P
 13228-37-0P 16885-94-2P 16885-99-7P 42951-62-2P 57662-47-2P
 76916-48-8P 76916-49-9P 76916-51-3P 76916-54-6P 76916-55-7P
 76916-57-9P 76916-58-0P 76916-60-4P 76916-63-7P 76916-67-1P

Garrett 10/729, 738

04/06/2005

76916-69-3P **76927-69-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

=>